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NAPAP (National Acid Precipitation Assessment Program) Emissions Inventory: Overview of Allocation Factors, 1985

Alliance Technologies Corp., Bedford, MA

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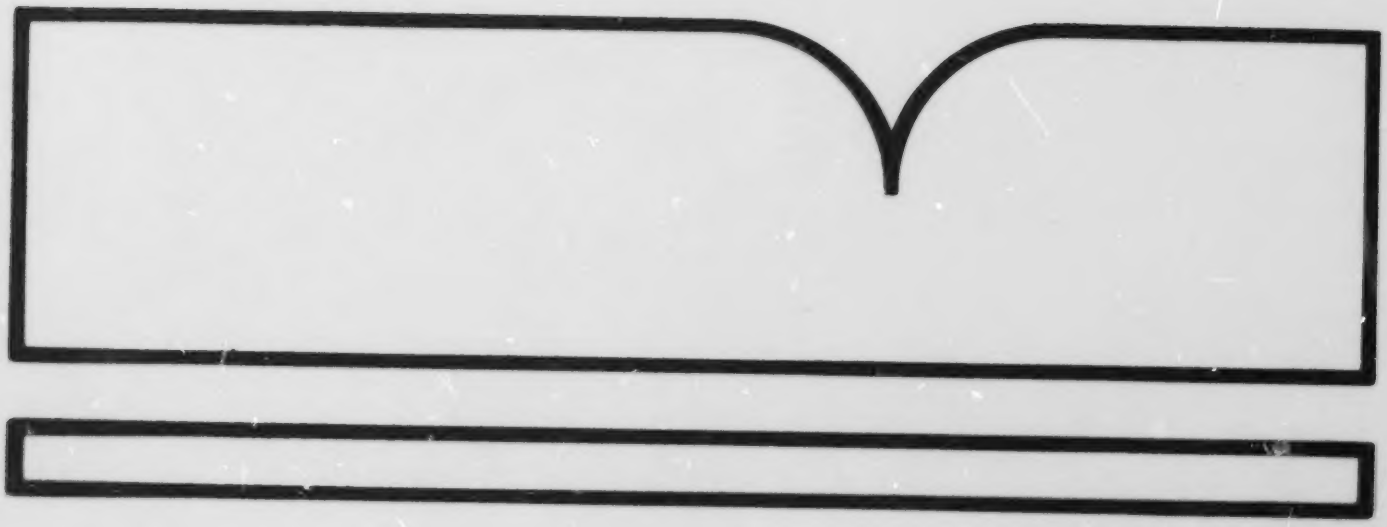

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THE 1985 NAPAP EMISSIONS INVENTORY: OVERVIEW OF ALLOCATION FACTORS

Prepared by

Robert A. Walters
Lysa G. Modica
David B. Fratt

ALLIANCE TECHNOLOGIES CORPORATION
213 Burlington Road
Bedford, Massachusetts 01730

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Robert C. Lagemann, EPA Project Officer
Air and Energy Engineering Research Laboratory
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711

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AIR AND ENERGY ENGINEERING RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
RESEARCH TRIANGLE PARK, NC 27711

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16. ABSTRACT

The report documents the development of temporal, spatial, and species allocation factors for the 1985 National Acid Precipitation Assessment Program (NAPAP) anthropogenic point and area source emissions inventories. These allocation factors are used to apportion annual emissions totals into gridded, hourly, speciated emissions estimates suitable for use as input to atmospheric transport models such as the Regional Acid Deposition Model. The temporal, spatial, and species allocation factors are discussed in detail in separate report sections. Each section contains a description of the methodology for application of the factors, a discussion of data sources, and documentation of the activities undertaken to create the allocation factor data sets used in the 1985 NAPAP resolved modeling inventories.

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FOREWORD

This report documents the development of allocation factors for the 1985 National Acid Precipitation Assessment Program (NAPAP) Emissions Inventories. As part of the NAPAP inventory development effort, EPA currently plans to publish additional reports which will address various elements of allocation factor development and application in greater detail:

The 1985 NAPAP Emissions Inventory (Version 2): Development of the Annual Data and Modeler's Tapes

An integrated report of the inventory development process, this document will contain sections on the development of the allocation factors as well as a description of the software used to apply the factors to annual emissions data.

The 1985 NAPAP Emissions Inventory: Development of Temporal Allocation Factors

This report will provide a detailed description of the data sources and methodologies used to develop and enhance the NAPAP temporal factors. It will also contain descriptions of data processing software and complete temporal factor listings.

The 1985 NAPAP Emissions Inventory: Development of Spatial Allocation Factors

This report summarizes spatial allocation factor development for U.S. and Canadian area sources and documents the pertinent software and peripheral files used to create the factors. It also contains detailed descriptions of the quality control checks undertaken and subsequent enhancements made to the factors.

The 1985 NAPAP Emissions Inventory: Development of Species Allocation Factors

This report will contain information on speciation methodologies for hydrocarbons, NO_x and particulate matter, and summarize computer programs and software used to generate speciation factors. Additional topics addressed in the report will include development of class-average molecular weights and hydrocarbon preprocessing.

Interested readers may wish to refer to these documents as they become available.

EPA REVIEW NOTICE

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ABSTRACT

The 1985 NAPAP Emissions Inventory has been developed by the National Acid Precipitation Assessment Program's (NAPAP) Task Group on Emissions and Controls. Temporal, spatial, and pollutant species allocation factors were developed to convert annual emissions data into resolved modeling formats to support the Regional Acid Deposition Model (RADM) and the Regional Oxident Model (ROM). The level of resolution required for the allocation factors was determined by the modelers based on analyses of model performance and emissions data bases. Allocation factors were originally developed for processing the 1980 NAPAP anthropogenic emissions inventory. These 1980 NAPAP allocation factors, and the methodologies developed, served as the basis for the 1985 allocation factor development.

Temporal allocation factors are comprised of three separate multipliers which permit resolution of annual emissions to the hourly level for a typical weekday, Saturday, or Sunday in each season. Spatial allocation factors apportion county-level area source emissions to modeling grid cells; point sources are assigned to grid cells based on location data. Speciation factors allow hydrocarbon emissions to be resolved into 32 representative chemical classes. NO_x emissions are resolved into NO and NO_2 and TSP emissions into 15 classes based on alkalinity and size distribution.

This report describes the allocation methodologies applied to convert the 1985 NAPAP Emissions Inventory annual data base into a resolved format suitable as input to the Regional Acid Deposition Model (RADM). The completion of the allocation process produced the 1985 NAPAP Modelers' Emissions Inventory Version 2. The Modelers' Inventory is being used as input to RADM for NAPAP assessment studies. This report is intended to provide an overview of the allocation factor data bases and allocation methodologies.

EXECUTIVE SUMMARY

This report documents the development of temporal, spatial, and species allocation factors for the 1985 National Acid Precipitation Assessment Program (NAPAP) anthropogenic point and area source emissions inventories. These allocation factors are used to apportion annual emissions totals into gridded, hourly, speciated emissions estimates suitable for use as input to atmospheric transport models such as the Regional Acid Deposition Model (RADM).

Resource and logistical constraints prevented the collection of daily emissions data for the entire base year of record (1985). Therefore, allocation factors have been developed to represent a typical weekday, Saturday and Sunday for each of the four seasons. The modelers inventory is divided into 12 temporal scenarios, one representing each of the day types. Each of the 12 scenarios is further resolved to the hourly level, for a total of 288 hourly values.

The RADM includes a chemical reaction mechanism to simulate the transformation of primary emissions into stable product species during transport. Emissions are reported in the annual inventory system as estimates of SO_2, NO_x, VOC, CO and TSP. Speciation factors are applied to the aggregated emissions such that the modeling inventory includes emissions estimates of NO_2 and NO, 32 chemical classes of hydrocarbons and three size fractions of four reactive components of alkaline particulate species in addition to SO_2, CO, SO_4, HF, HCL, AND NH_3. The grid pattern used to distribute the emissions data is defined by grids that are 1/4 degree longitude by 1/6 degree latitude (approximately 20 km by 20 km). There are 63,000 grid cells in the NAPAP grid system, including Canada.

Allocation factors are statistical representations of the spatial and temporal distribution of annual emissions, or representative speciation profiles for particular source types. Factors are generally applied to NAPAP annual emissions records on the basis of point source SCC (Source Classification Code) or NAPAP area source category.

The temporal, spatial, and species allocation factors are discussed in detail in separate report sections. Each section contains a description of the methodology for application of the factors, a discussion of data sources, and documentation of the activities undertaken to create the allocation factor data sets used in the 1985 NAPAP resolved modeling inventories.

TEMPORAL ALLOCATION FACTORS

In support of modeling applications, the annual emissions totals must be resolved temporally into 24 hourly totals for a typical weekday, Saturday or Sunday in each of the four seasons of the year. The NAPAP temporal allocation factors were developed to accomplish this resolution.

Temporal factors were created for U.S. point and area source emissions categories in the NAPAP inventories. Factors for the 1985 NAPAP inventory were derived primarily from temporal factors developed for the 1980 NAPAP effort. They reflect data from a variety of sources, which include previous modeling studies, as well as enhancements deemed necessary as part of the ongoing development of the NAPAP inventories.

Factors were developed for each of the 97 U.S. area source categories included in the 1985 inventories. In most cases, temporal allocation of point source data is accomplished using operating schedule information provided with the emissions records. However, given the magnitude of emissions from electric utilities, process-level (fuel and state specific) factors were developed from data supplied by the Department of Energy and Tennessee Valley Authority to more accurately characterize these sources.

Efforts to enhance the accuracy of temporal allocation are ongoing. Factor normalization has eliminated summation errors which occurred in previous inventories when temporally apportioned emissions were reaggregated. Other modifications included the incorporation of data sources which enhance the accuracy of temporal allocation.

SPATIAL ALLOCATION FACTORS

Spatial allocation factors were developed to apportion area source emissions from counties to individual grid cells as required for modeling applications. The actual spatial distribution of emissions are estimated according to the distribution of surrogate indicators. Fourteen such indicators were developed for use with the NAPAP inventory based on housing, population, and land-use data. For the 1985 NAPAP application, 6 of the 14 surrogates are used for spatial allocation.

To assure the quality and representativeness of the spatially resolved 1985 area source inventory, extensive quality control checks were performed on the existing spatial factors. Quality control procedures were both data and software intensive. Data analyses focused on evaluating spatial factors at the county level and ensuring the quality of national-, state-, and SCC-level gridded emissions totals. Software-intensive evaluations included reviewing computer code and implementing modifications to the spatial factor software for other applications. Based on the results of the quality control procedures, adjustments were made to the spatial factors and the computer programs. Once the adjustments were made, additional quality control checks were performed to assure the quality of the modified spatial factors.

SPECIATION FACTORS

Several of the pollutants in the 1985 NAPAP annual inventory represent composites of various individual species. To accommodate RADM requirements, annual hydrocarbon emissions estimates are split into 32 chemical species classes, annual NO_x estimates are divided into NO_2 and NO, and TSP emissions are resolved into 15 classes based on alkalinity and size fraction.

The hydrocarbon and particulate matter speciation factors were based on profiles developed by the U.S. EPA (Shareef et al., 1988). Percentage splits for NO and NO_2 were based on factors taken from AP-42 (U.S. EPA, 1985). A default split of 95 percent NO and 5 percent NO_2 was applied to processes that were not expected to be major NO_x sources. Specific species-class assignments for VOC were developed by the National Center for Atmospheric Research (NCAR). Alliance obtained these data, performed quality assurance checks, and developed software to convert the files into a format suitable for use with the 1985 NAPAP inventory processing software. Hydrocarbon species data were also used to create files for the preprocessing of VOC and THC to adjust for the presence of formaldehyde and methane in some NEDS emissions estimates.

SECTION 1
INTRODUCTION

BACKGROUND

The "Acid Precipitation Act of 1980" (Title VII of P.L. 96-294) established a long-term interagency program to coordinate and expand research on the problems posed by acid deposition in and around the United States. Among the priority research objectives that Congress identified for the National Acid Precipitation Assessment Program (NAPAP) was the development of a comprehensive nationwide inventory of emissions sources thought to contribute to the formation of acid rain. Complete and accurate inventories of acid deposition precursor emissions are necessary to support assessment activities and studies of source-receptor relationships using atmospheric process models. The NAPAP Task Group on Emissions and Controls has undertaken this objective by developing inventories of acid deposition precursor emissions for the base year 1985. The Environmental Protection Agency Office of Research and Development is responsible for developing the NAPAP emissions inventories.

The 1985 NAPAP anthropogenic inventories were developed in two phases. The first phase involved data collection and quality assurance of source characteristics and emissions totals on an annual basis (Zimmerman, et al., 1988). The data collection effort used as a basis the existing Environmental Protection Agency (EPA) National Emissions Data System (NEDS). NEDS data were supplemented by the application of noncriteria pollutant emission factors to yield a final data base of 10 pollutants (SO_2, SO_4, NO_x, TSP, CO, NH_3, HCl, HF, VOC, and total hydrocarbons).

The second phase of the inventory development involved the generation of a resolved emissions inventory containing gridded, hourly, and speciated emissions data. The spatial, temporal, and species allocation of the annual emissions totals are required to render the data suitable as input to regional atmospheric process models. For example, the Regional Acid Deposition Model (RADM), the principal model developed by NAPAP, is an event-specific analysis tool that requires specific daily inputs of meteorological and emissions data to simulate deposition episodes.

Resource and logistics constraints precluded the collection of sufficiently resolved emissions data for the entire base year of record (1985). For example, to collect hourly emissions data for each 1/4 degree longitude by 1/6 degree latitude grid cell for each of the 59 species would be a monumental task at best. Therefore, a set of allocation factors was developed to resolve annual emissions data, using statistical representations of the

spatial and temporal distribution of annual emissions and representative speciation profiles for particular source types. The level of resolution of the allocation factors have been determined by the modelers based on analyses of model performance and emissions data bases (Middleton, 1987).

Temporal allocation factors are comprised of three separate multipliers: seasonal, daily and hourly. Spatial allocation factors apportion county-level area source emissions to modeling grid cells; point sources are assigned to grids cells based on location data (e.g., latitude and longitude or Universal Transverse Mercator (UTM) coordinates). Speciation factors allow hydrocarbon emissions to be resolved into 32 representative chemical classes. NO_x emissions are resolved into NO and NO_2, and TSP emissions are resolved into 15 classes on the basis of alkalinity and size distribution.

The temporal, spatial, and species allocation data were used as input to the Flexible Regional Emissions Data System (FREDS) (Modica, et al., 1989), which matches the annual process-level emissions with appropriate allocation factors to derive the gridded, hourly, speciated emissions estimates required for RADM input. Version 1 of the point and area source modeling inventories generated by FREDS was delivered to EPA in September 1988.

SUMMARY

Allocation factors were originally developed for processing the 1980 NAPAP anthropogenic emissions inventory (Sellars, et al., 1985). These factors, and the methodologies developed for assigning them to emissions records, formed the starting point for the 1985 allocation factor development effort. Following the completion of the 1980 inventory, the methods, data, and documentation used to develop allocation factors were examined.

Limitations were identified, the availability of new data was investigated, and requirements as to the necessity and extent of changes to existing allocation factors were determined. In particular, updated hydrocarbon and particulate speciation data became available and were used to create entirely new speciation factors. Temporal and spatial factors remained largely based on data gathered for the 1980 inventory.

The 1985 NAPAP inventory contains county-level emission estimates for several area source categories not included in previous inventories (Demmy, et al., 1988). In some cases, these new source types could be accurately characterized by application of existing allocation data. Where this was not possible, new profiles were developed. Additional issues were noted and addressed on a case-by-case basis. For example, a county in New Mexico which was formed after 1980, had no corresponding spatial data in the original files, and required a reapportionment of land area to account for its presence.

In addition, to ensure the quality of the resolved emissions estimates, extensive quality control checks were performed both on the new factors and those adopted from the 1980 data base, and corrections were made accordingly. The computer programs used to process the allocation data into a format suitable for use with FREDS were also tested and checked for errors in logic or data format.

REPORT ORGANIZATION

The remainder of this report documents the development of the various allocation factors for the 1985 NAPAP anthropogenic point and area source inventories. Section 2 provides a discussion of the temporal factor development from a current and historical perspective. In Section 3, spatial factor development and processing requirements are detailed. Section 4 provides information on the development of hydrocarbon, NO_x and particulate speciation factors. Each of these three sections includes background information on the application of the factors, a discussion of data sources, and a description of the activities undertaken to create allocation factor data sets suitable for use with the NAPAP inventory. Each section also contains a brief description of the allocation factor files and computer formats as used by FREDS to create a resolved modeling inventory. References, contained in Section 5, are organized by allocation factor type to facilitate the identification of relevant documentation.

SECTION 2

TEMPORAL ALLOCATION FACTORS

INTRODUCTION

In support of modeling applications, annual emissions totals must be resolved temporally into 24 hourly totals for a typical weekday, Saturday and Sunday in each of the four seasons of the year. To accomplish this task, seasonal, daily, and hourly allocation factors were developed and applied to NAPAP point and area source data.

The temporal allocation factors take the form of three sets of fractional multipliers, applied to the NAPAP annual emissions records in sequence as follows:

1. Four seasonal factors divide the annual total into four subtotals representing emissions in each season.
2. Three daily factors per season divide each seasonal total into three subtotals representing emissions for a typical weekday, Saturday and Sunday in each season.
3. Twenty-four hourly factors per day divide each daily total into 24 subtotals representing emissions for each hour of that day. After this final step, the annual emissions have been divided into 288 subtotals (four seasons x 3 day "types"/season x 24 hrs/day "type").

The seasonal multipliers for each record sum to unity, as do the hourly multipliers for each season/day type combination. Since daily emissions totals represent emissions for one typical weekday, Saturday or Sunday in each season, the governing equation for daily allocation factors is:

$$(65 \times \text{weekday factor}) + (13 \times \text{Saturday factor}) + (13 \times \text{Sunday factor}) = 1 \qquad (2.1)$$

where a season is defined as 91 days (13 weeks). For the purposes of the NAPAP inventory, the four seasons are defined as:

Season	Months
Winter	December, January, February
Spring	March, April, May
Summer	June, July, August
Fall	September, October, November

All temporal factors are defined according to local time (e.g., the factor for "Hour 1" corresponds to the period between midnight and 1:00 a.m., local time). However, modeling applications require that these factors be offset to Greenwich Mean Time (GMT) to produce standardized allocation for all U.S. sources. Offset to GMT is accomplished during processing of the annual emissions inventories by integrating local factors with time zone information. Where appropriate, additional data adjust the factors for Daylight Savings Time.

Temporal allocation factors were developed for U.S. point and area source categories in the NAPAP inventory. The factors reflect data from a variety of sources, including previous modeling studies. Many of the factors are based on data from the Northeast Corridor Regional Modeling Project (NECRMP). In the NECRMP effort, estimates of temporal patterns were developed for point and area source emissions in 15 States in the eastern United States. Factors from the NECRMP States were often retained for the NAPAP inventories; other factors were developed for states outside the NECRMP study area.

Point-specific factors were developed for only a subset of all point sources. Specifically, temporal profiles were derived for electric utility processes, as they are among the largest emitters of acid rain precursors. In most cases, however, temporal allocation of point-source emissions was estimated using operating schedule information provided with annual emissions records.

Where specific temporal factors were not developed, emissions are allocated uniformly during processing of the NAPAP point and area source data. The following default profiles are used:

Factor Type	Uniform Default Value
Seasonal	1/4
Daily	1/91
Hourly	1/24

AREA SOURCE TEMPORAL ALLOCATION FACTORS

Temporal factors were developed for the 102 source categories in the NAPAP area source file. Depending on the magnitude of emissions within the category and the availability of data, temporal factors were frequently resolved to the State or regional level (i.e., different sets of factors for each State and county for a given source category). A complete list of area source categories used in the 1985 NAPAP inventories, including the level of resolution for each SCC-specific temporal pattern is provided in Table 2-1.

A description of the development of area source factors for each category or set of categories follows. Categories which were recently added or factors which have been modified for the 1985 NAPAP effort are noted in the text. Categories added for the 1985 inventories include:

TABLE 2-1. SOURCE CATEGORIES FOR U.S. AREA SOURCES, 1985 NAPAP INVENTORY

Category No.	Category description	Level of temporal factor resolution
1	Residential Fuel - Anthracite Coal	STATE
2	Residential Fuel - Bituminous Coal	STATE
3	Residential Fuel - Distillate Oil	STATE
4	Residential Fuel - Residual Oil	STATE
5	Residential Fuel - Natural Gas	STATE
6	Residential Fuel - Wood	STATE
7	Commercial/Institutional Fuel - Anthracite Coal	STATE (NECRMP STATES), NATIONAL (OTHER)
8	Commercial/Institutional Fuel - Bituminous Coal	STATE (NECRMP STATES), NATIONAL (OTHER)
9	Commercial/Institutional Fuel - Distillate Oil	STATE (NECRMP STATES), NATIONAL (OTHER)
10	Commercial/Institutional Fuel - Residual Oil	STATE (NECRMP STATES), NATIONAL (OTHER)
11	Commercial/Institutional Fuel - Natural Gas	STATE (NECRMP STATES), NATIONAL (OTHER)
12	Commercial/Institutional Fuel - Wood	STATE (NECRMP STATES), NATIONAL (OTHER)
13	Industrial Fuel - Anthracite Coal	NATIONAL
14	Industrial Fuel - Bituminous Coal	NATIONAL
15	Industrial Fuel - Coke	NATIONAL
16	Industrial Fuel - Distillate Oil	NATIONAL
17	Industrial Fuel - Residual Oil	NATIONAL
18	Industrial Fuel - Natural Gas	NATIONAL
19	Industrial Fuel - Wood	NATIONAL
20	Industrial Fuel - Industrial Process Gas	NATIONAL
21	Incineration - Residential	NATIONAL
22	Incineration - Industrial	NATIONAL
23	Incineration - Commercial/Institutional	NATIONAL
24	Open Burning - Residential	NATIONAL
25	Open Burning - Industrial	NATIONAL
26	Open Burning - Commercial/Institutional	NATIONAL
27	Light Duty Gas Vehicles - Limited Access Roads	NATIONAL
28	Light Duty Gas Vehicles - Rural Roads	NATIONAL
29	Light Duty Gas Vehicles - Suburban Roads	NATIONAL
30	Light Duty Gas Vehicles - Urban Roads	NATIONAL
31	Medium Duty Gas Vehicles - Limited Access Roads	NATIONAL
32	Medium Duty Gas Vehicles - Rural Roads	NATIONAL
33	Medium Duty Gas Vehicles - Suburban Roads	NATIONAL
34	Medium Duty Gas Vehicles - Urban Roads	NATIONAL
35	Heavy Duty Gas Vehicles - Limited Access Roads	NATIONAL
36	Heavy Duty Gas Vehicles - Rural Roads	NATIONAL
37	Heavy Duty Gas Vehicles - Suburban Roads	NATIONAL
38	Heavy Duty Gas Vehicles - Urban Roads	NATIONAL
39	Off-Highway Gas Vehicles	STATE
40	Heavy Duty Diesel Vehicles - Limited Access Roads	NATIONAL
41	Heavy Duty Diesel Vehicles - Rural Roads	NATIONAL
42	Heavy Duty Diesel Vehicles - Suburban Roads	NATIONAL
43	Heavy Duty Diesel Vehicles - Urban Roads	NATIONAL
44	Off-Highway Diesel Vehicles	STATE
45	Railroad Locomotives	REGION
46	Aircraft - Military	NATIONAL
47	Aircraft - Civil	NATIONAL
48	Aircraft - Commercial	NATIONAL
49	Vessels - Coal	NATIONAL
50	Vessels - Diesel	NATIONAL
51	Vessels - Residual Oil	NATIONAL
52	Vessels - Gasoline	STATE
53*	Solvents Purchased (not used)	
54	Gasoline Marketed	NATIONAL
55	Unpaved Road Travel	NATIONAL
56	Unpaved Airport LTOs	NATIONAL
57	(Not used)	
58	(Not used)	
59	(Not used)	
60	Forest Fires	NATIONAL

(continued)

TABLE 2-1 (continued)

Category No.	Category description	Level of temporal factor resolution
61	Managed Burning - Prescribed	NATIONAL
62	Agricultural Field Burning	NATIONAL
63	(Not used)	
64	Structural Fires	NATIONAL
65	(Not used)	
66	Ammonia Emissions - Light Duty Gasoline Vehicles	NATIONAL
67	Ammonia Emissions - Heavy Duty Gasoline Vehicles	NATIONAL
68	Ammonia Emissions - Heavy Duty Diesel Vehicles	NATIONAL
69**	Livestock Waste Management - Turkeys	REGION
70**	Livestock Waste Management - Sheep	REGION
71**	Livestock Waste Management - Beef Cattle	REGION
72**	Livestock Waste Management - Dairy Cattle	REGION
73**	Livestock Waste Management - Swine	REGION
74**	Livestock Waste Management - Broilers	NATIONAL
75**	Livestock Waste Management - Other Chickens	NATIONAL
76	Anhydrous Ammonia Fertilizer Application	REGION
77	Beef Cattle Feed Lots	NATIONAL
78	Degreasing	NATIONAL
79	Drycleaning	NATIONAL
80	Graphic Arts/Printing	NATIONAL
81	Rubber and Plastics Manufacturing	NATIONAL
82	Architectural Coating	NATIONAL
83	Auto Body Repair	NATIONAL
84	Motor Vehicle Manufacture	NATIONAL
85	Paper Coating	NATIONAL
86	Fabricated Metals	NATIONAL
87	Machinery Manufacture	NATIONAL
88	Furniture Manufacture	NATIONAL
89	Flatwood Products	NATIONAL
90	Other Transportation Equipment Manufacture	NATIONAL
91	Electrical Equipment Manufacture	NATIONAL
92	Ship Building and Repairing	NATIONAL
93	Miscellaneous Industrial Manufacture	NATIONAL
94***	(Not used)	NATIONAL
95***	Miscellaneous Solvent Use	NATIONAL
96	Minor Point Sources-Coal Combusiton	NATIONAL
97	Minor Point Sources-Oil Combustion	NATIONAL
98	Minor Point Sources-Natural Gas Combustion	NATIONAL
99	Minor Point Sources-Process Sources	NATIONAL
100	Publicly-Owned Treatment Works (POTWs)	NATIONAL
101	Cutback Asphalt Paving Operation	NATIONAL
102	Fugitives from Synthetic Organic Chemical Manufacture	NATIONAL
103	Bulk Terminal and Bulk Plants	NATIONAL
104	Fugitives from Petroleum Refinery Operations	NATIONAL
105	Process Emissions from Bakeries	NATIONAL
106	Process Emissions from Pharmaceutical Manufacture	NATIONAL
107	Process Emissions from Synthetic Fibers Manufacture	NATIONAL
108	Crude Oil and Natural Gas Production Fields	NATIONAL
109	Hazardous Waste Treatment, Storage, and Disposal Facilities (TSDFs)	NATIONAL

NECRMP STATES: Connecticut, Delaware, District of Columbia, Maine, Maryland, Massachusetts, New Hampshire, New Jersey, New York, Ohio, Pennsylvania, Rhode Island, Vermont, Virginia, West Virginia.

* - Category 59 is disaggregated into process categories 78 to 95.

** - These categories formerly referred to as "manure field application."

*** - Formerly "miscellaneous industrial solvent use" (94) and "miscellaneous non-industrial solvent use" (95); now combined into one category (95).

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- Ammonia Emissions - Vehicular Sources (Categories 66-68);
- Livestock Waste Management (Categories 69, 70); and
- Miscellaneous VOC Categories (Categories 100-109).

Residential Fuel Combustion (Categories 1-6)

The residential fuel categories account for emissions from residential water heating, space heating, and cooking. The surrogate for the temporal variability in emissions is heating degree days, which reflects variability in average temperature.

To develop state-specific seasonal factors, monthly average heating degree days for each state for 1980 were obtained from *State, Regional, and National Monthly and Seasonal Heating Degree Days Weighted by Population* (U.S. Department of Commerce, 1983b). For each month, temperature averages were calculated for state climatic divisions, which are regions within a state that are considered to be climatically homogeneous. Monthly heating degree day totals for each division were calculated from the monthly mean temperature. State-level average degree day totals for each month were derived from divisional values by weighting each division by its percentage of total state population, as obtained from the 1980 Census; degree day totals were therefore biased toward areas of the state having the greatest population. Seasonal temporal factors were developed by determining the fractional distribution of annual heating degree days by month and summing over each season.

Since the variability of residential heating emissions is assumed to be dependent only on temperature, a uniform daily temporal pattern was assigned in the NAPAP effort. The hourly variations in residential fuel use were developed with data from NOAA (U.S. Department of Commerce, 1980). Monthly averages of 3-hour meteorological records were obtained for a representative meteorological station in each state. For each month, the averaged 3-hour temperatures were subtracted from 18.7°C (65°F), which is the value used to calculate degree days. Negative values (indicating temperatures above 18.7°C) were set to zero. The resulting eight values were proportional to the variation in diurnal heating for a selected station for a month. Months were then averaged to obtain seasonally adjusted diurnal factors for each state.

Commercial/Institutional Fuel Combustion (Categories 7-12)

Area source emissions from fuel use by commercial and institutional sources consist of emissions from all fuel burned in stationary sources that are not included under residential sources, industrial sources, power plants or commercial point sources.

Seasonal allocation factors were developed from *Procedures for the Preparation of Emission Inventories for Volatile Organic Compounds, Volume II* (EPA, 1979b), hereafter referred to as the EPA Guidelines. These

Guidelines recommend that 25 percent of emissions be spread uniformly across the seasons, and that the remaining 75 percent be uniformly allocated to those months in which the average temperature is 18.7°C (65°F) or less. The seasonal splits in the temporal allocation factors presented in NAPAP are 35 percent winter, 25 percent spring, 15 percent summer, and 25 percent fall.

EPA Guidelines were also used to generate daily temporal factors. The Guidelines recommend that 95 percent of emissions be uniformly allocated from Monday through Saturday, and 5 percent be allocated to Sunday. For NAPAP, it was thought that too little of the emissions were allocated to Sunday, since a certain amount of energy is needed to keep buildings at an acceptable temperature. The revised profile allocates 90 percent of emissions uniformly from Monday through Saturday, and the remaining 10 percent to Sunday.

Hourly patterns for commercial/institutional fuel use for NECRMP states were taken from the NECRMP study data. This pattern was developed in the Philadelphia AQCR inventory effort (Engineering-Science, 1982). The profile assumes that 50 percent of daily emissions are released uniformly from 7:00 a.m. to 4:00 p.m., with the other 50 percent released during the remaining hours in the day. Outside the NECRMP area, hourly allocation factors were taken from the EPA Guidelines, which indicate 90 percent of emissions are released between 5:00 a.m. and 10:00 p.m., and 10 percent during the remaining hours in the day.

Industrial Fuel Combustion (Categories 13-20)

These categories include emissions from the industrial sector which are not accounted for by point source categories. National seasonal patterns were developed from the EPA Guidelines (EPA, 1979b), in which a uniform distribution is recommended.

The daily pattern was based on U.S. Bureau of Labor statistics on average overtime at manufacturing facilities (U.S. Department of Labor, 1981). All overtime hours were assumed to be worked on weekends, and three times as much overtime was worked on Saturdays as on Sundays. The daily pattern developed from these data indicate that approximately 93 percent of emissions are produced on weekdays, 5 percent on Saturdays, and 2 percent on Sundays.

The hourly pattern was taken from NECRMP (Sellars, et al., 1982), and was developed during the Philadelphia AQCR inventory effort (Engineering-Science, 1982). Fifty percent of industrial coal and oil fuel use emissions were allocated uniformly from 7:00 a.m. to 4:00 p.m., to reflect greater production during business hours. The remaining 50 percent of emissions were uniformly allocated to the remaining hours in a day.

Onsite Incineration and Open Burning (Categories 21-26)

For the purposes of determining solid waste generated, onsite incineration is defined as disposal in a small incinerator. Using this definition, incineration encompasses the following types of disposal units: backyard burners, industrial incinerators, and incinerators used by food and department stores, hospitals, and schools. Since large municipal incinerators are usually classified as point sources, emissions resulting from disposal in this type of incinerator have not been included in this category. For the purposes of estimated open burning practices, open burning refers to uncombined burning of wastes such as leaves, landscape refuse, and other rubbish. Large open burning dumps are usually included under point sources. Both onside incineration and open burning categories are considered separately in NAPAP for the residential, commercial/institutional, and industrial sectors.

A single temporal profile set, developed in the NECRMP effort, was assigned to these categories on a national level. The profile assumes that emissions occur uniformly throughout the year. The daily pattern assumes that 91 percent of emissions are produced on weekdays, and 9 percent are generated on Saturdays. The hourly factors allot emissions uniformly from 6:00 a.m. to 5:00 p.m. NECRMP documentation indicates that this profile was based on temporal data in the St. Louis RAPS effort (EPA, 1979a), the Tulsa, OK inventory (EPA, 1980), and data from the states of New Jersey and New York (Sellars et al, 1982).

Highway Vehicles, Light and Medium Duty (Categories 27-34)

These eight categories account for exhaust and tire wear emissions from automobiles and light trucks (0-8,500 lb gross vehicle weight [GVW]) on limited access, rural, suburban and urban roads. National-level factors were developed for each of these eight categories, using data obtained from the U.S. Department of Transportation (Welty, K. personal communication. Mr. Welty supplied traffic statistics compiled by the Highway Statistics Division, Federal Highway Administration, U.S. Department of Transportation, on a diskette formatted for use on an IBM Personal Computer.) These data were analyzed with FORTRAN software designed specifically to calculate temporal allocation factors in the format required by the FREDS data processing system. This agency collects continuous traffic count data from all 50 states, and uses a subset of these data covering 12 states as a basis for estimating national traffic patterns. Data from these 12 states allow hourly temporal allocation factors to be derived for each day of the week in each month of the year for six roadway types: rural and urban Interstate, rural and urban other arterial, and rural and urban collector/local. This data set was obtained and analyzed to yield seasonal, daily, and hourly temporal allocation factors for light and medium duty vehicles. The pattern for limited access roads was derived from an analysis of the rural and urban Interstate groups; the pattern for rural roads was taken from an analysis of the rural other arterial group; and the pattern for suburban and urban roads resulted from an analysis of the urban other arterial group.

Heavy Duty Highway Vehicles (Categories 35-38, 40-43)

These categories account for emissions from gasoline and diesel trucks weighing more than 8,500 lb GVW. Emissions from these vehicles are inventoried separately for limited access roads, rural roads, suburban roads and urban roads. A uniform seasonal pattern has been assigned to all these categories, after its applicability was confirmed by the U.S. Trucking Association (Sellars et al, 1985).

A lack of daily factor data necessitated a uniform daily split for the Heavy Duty Gasoline Vehicle (HDGV) and Heavy Duty Diesel Vehicle (HDDV) truck categories. The hourly profile for HDGV and HDDV was derived from NECRMP data and was based on a profile developed for the Philadelphia AQCR inventory effort (Engineering-Science, 1982). Although not explicitly stated in the Philadelphia report, it is likely that these data were compiled by the Delaware Valley Regional Planning Commission (DVRPC) and documented in a 1982 report. (Delaware Valley Highway Vehicle Emissions Inventory, September 1982).

Off-Highway Vehicles (Categories 39,44)

The off-highway vehicle area source categories account for gasoline and diesel emissions generated by farm equipment, construction equipment, industrial equipment, motorcycles, lawn and garden equipment, and snowmobiles. Seasonal patterns for the off-highway vehicle categories were derived from data contained in *Highway Statistics* (U.S. Department of Transportation, 1980). For this effort, monthly distributions of off-highway motor vehicle fuel use were calculated on a state-specific basis by subtracting monthly on-highway fuel use from total monthly fuel use. state-specific seasonal patterns were then derived from the monthly data.

Daily patterns were derived from the EPA Guidelines (EPA, 1979b), and are a composite (weighted by emission strength) of the daily patterns for five subcategories of off-highway vehicles (agricultural equipment, construction equipment, industrial equipment, lawn and garden equipment, and motorcycles) for which factors are separately described in the Guidelines. The suggested daily patterns for each subcategory are as follows:

- **Farm equipment** - uniform through the week
- **Construction equipment** - uniform Monday through Saturday
- **Industrial equipment** - uniform Monday through Saturday
- **Lawn and garden equipment** - 50 percent Monday through Friday, 50 percent Saturday through Sunday
- **Off-highway motorcycles** - 30 percent Monday through Friday, 70 percent Saturday through Sunday
- **Snowmobiles** - 30 percent Monday through Friday, 70 percent Saturday through Sunday

The resulting weighted daily pattern assigns emissions uniformly over the week.

The NECRMP documentation describes the development of separate hourly patterns for gasoline and diesel vehicles, as follows. First, a single hourly pattern was developed for the composite of five of the component subcategories identified previously. Next, percentages of gasoline and diesel usage were derived for the five subcategories of off-highway use with information obtained from *Highway Statistics, 1980* (U.S. Department of Transportation, 1980) (Table MF-24), "Private and Commercial Non-Highway Use of Gasoline" and a combination of material from various NECRMP area source emission inventories (Ohio, Virginia, New Hampshire, and Delaware) (Sellars, et al., 1982). These weighted percentages were then applied to the composite hourly curve to produce composite curves for gasoline and diesel off-highway fuel use.

Railroads (Category 45)

This category accounts for emissions from locomotives and fuel used by railroad stations and workshops for space heating. The latter fuel consumption was included primarily because it is difficult to separate from total railroad fuel use; railroad space heating emissions are considered insignificant compared to those generated by locomotive fuel consumption (Sellars, et al., 1982).

Within the NECRMP region, temporal patterns for locomotives were based on information provided by Conrail for the Philadelphia AQCR inventory effort (Engineering-Science, 1982). Most emissions in this category are due to freight service rather than passenger service. A sales manager at Conrail indicated that 36 percent of the traffic occurred uniformly between 5:00 p.m. and 11:00 p.m. EST, and the remaining 64 percent was equally distributed around the clock. Midday local traffic involved the movement of boxcars for loading and unloading. No seasonal variations were assumed. The Conrail sales manager indicated there was only a slight weekday-weekend day preference, so an operating schedule based on a 6.3-day work-week was assumed.

Outside the NECRMP region, temporal patterns were developed according to EPA Guidelines (EPA, 1979b). The Guidelines recommend uniform emissions throughout the year and week, with 70 percent of hourly emissions being generated from 7:00 a.m. to 6:00 p.m. and 30 percent from 6:00 p.m. to 7:00 a.m.

Aircraft (Categories 46-48, 56)

Aircraft are divided into civil, military and commercial subgroups in the NAPAP inventory. For civil aircraft, seasonal daily and hourly patterns were derived from the EPA Guidelines (EPA, 1979b). A uniform seasonal distribution is recommended, with 40 percent of operations occurring on weekends and 60 percent on weekdays. Emissions are allocated uniformly from 7:00 a.m. to 9:00 p.m.; levels outside this period are set to zero. The same temporal profile was used to allocate emissions from unpaved airport LTOs (Category 56).

For military aircraft, patterns were derived from the Philadelphia AQCR Inventory (Engineering-Science, 1982). Interviews from this study led to the adoption of a uniform seasonal and daily pattern for military aircraft, with 55 percent allocated between 9:00 a.m. and 9:00 p.m., and 45 percent spread uniformly over the remaining hours. For commercial aircraft, seasonal patterns were derived from unpublished data presented in the U.S. Civil Aeronautics Board (CAB)'s *Seasonally Adjusted Traffic and Capacity*. The CAB report provided national statistics on monthly domestic traffic handled by the major air carriers. Commercial aircraft emissions were assumed to occur 7 days/week, with 90 percent of all commercial emissions occurring between 6:00 a.m. and midnight.

Vessels (Categories 49-52)

Emissions from vessels are split into four area source categories on the basis of fuel type. Coal-, diesel-, and residual fuel-powered vessels include large river- and ocean-going barges. Gasoline-powered vessels are mostly for recreational use. Temporal patterns for all vessels were developed from the EPA Guidelines (EPA, 1979b). The following patterns were used:

- **Ocean and river cargo vessels**

  Seasonal—uniform

  Daily—uniform

  Hourly—75 percent from 7:00 a.m. to 7:00 p.m. and
  25 percent from 7:00 p.m. to 7:00 a.m.

- **Pleasure craft**

  Seasonal—uniform during months with an average temperature of 45°F or higher.

  Daily—30 percent Monday through Friday, 70 percent Saturday through Sunday

  Hourly—uniform from 7:00 a.m. to 6:00 p.m., otherwise zero

The seasonal patterns for pleasure craft were developed using State-level average temperature data compiled by the NOAA (U.S. Department of Commerce, 1983a).

Gasoline Marketing (Category 54)

This area source category accounts for emissions from tanker truck loading and transit, gasoline station loading, storage tank breathing and vehicle fueling. Sources investigated in the development of seasonal patterns were refiner sales to end users, and consumption data from the U.S. Department of Energy's (DOE's) *Petroleum Marketing Monthly* (U.S. DOE, 1984) and the U.S. Department of Transportation's *Highway Statistics 1980* (U.S. Department of Transportation, 1980). From analyses of these data, it was concluded that

the evidence was insufficient to justify using other than a uniform seasonal distribution. Daily and hourly patterns were based on the EPA Guidelines (EPA, 1979b) which indicate uniform emissions Monday through Saturday, with uniform emissions from 6:00 a.m. to 8:00 p.m., and no emissions at other times.

Unpaved Roads (Category 55)

The seasonal, daily and hourly patterns for this category were taken from those for light duty vehicles on rural roads.

Forest Fires (Category 60)

Forest fires were assumed to occur randomly, 7 days per week, 24 hours per day. It was estimated that 90 percent of forest fires occur during summer or fall, and that the remaining 10 percent are split evenly between winter and spring.

Agricultural Burning (Categories 61 and 62)

Both of these categories were assigned the patterns developed for field/slash burning in the NECRMP study (Sellars, et al., 1982). The NECRMP pattern assumed burning to occur 7 days per week, and uniformly between 5:00 a.m. and 8:00 p.m. It was also assumed that no burning would occur during the summer season. The actual NAPAP seasonal splits are 10 percent winter, 70 percent spring, 0 percent summer, and 20 percent fall.

Structural Fires (Category 64)

Structural fires are assumed to occur randomly throughout the year. Thus a uniform seasonal, daily and hourly pattern was assumed for this category.

Ammonia Emissions - Vehicular Sources (Categories 66-68)
(Added for 1985 NAPAP Inventory)

These new categories contain ammonia emissions for three vehicle types: light-duty gasoline, heavy-duty gasoline, and heavy-duty diesel. Temporal profiles were taken directly from corresponding urban vehicular categories for which emissions of other pollutants were reported (Categories 30, 38, and 43, respectively).

Livestock Waste Management (Categories 69-75)
(SCCs 69 and 70 added for 1985 NAPAP inventory)

Ammonia emissions from livestock waste management include those resulting from production and field application of different types of livestock manure. Emissions for these categories were estimated on the basis of number of each type of livestock, weighted to account for the percentage confined and unconfined animals.

National-level temporal patterns were generally uniform for seasonal, daily, and hourly allocation. To establish state-level profiles Agricultural Extension Agents in 12 states across the country (Indiana, Wisconsin, Nebraska, Kansas, North Dakota, Idaho, Iowa, North Carolina, Alabama, New York, Texas and Arkansas) were contacted; they provided information on the patterns of manure application in their states. These patterns were extended to nearby states not contacted directly.

For the 1985 effort, emissions for turkey and sheep waste management (Categories 69 and 70) were provided in addition to the livestock categories reported previously (Categories 71-75). Temporal profiles for these new sources were assumed to be similar to those used for other livestock waste management categories, and were copied directly from Category 71 (beef cattle waste management).

NH_3 Fertilizer Application (Category 76)

The 12 Agricultural Extension Agents contacted to provide information on manure-spreading practices (see above) were also asked to share their knowledge of NH_3 fertilization practices. Daily factors were derived from the assumption that no fertilizer application occurs on Sundays; the national daily pattern assigns emissions uniformly Monday through Saturday. The national hourly pattern assumes approximately 60 percent of emissions occur between 8:00 a.m. and 7:00 p.m., 17 percent occur between 9:00 p.m. and 4:00 a.m., and the remainder are distributed over the intervening period (Wagner et al, 1986).

Beef Cattle Feed Lots (Category 77)

Emissions were allocated according to uniform seasonal, daily, and hourly patterns.

Solvent Use Categories (Categories 78-95)

Early versions of the NAPAP area source inventories reported a large composite category (53) for organic solvent evaporation based on data from NEDS. Certain NEDS-generated reports, however, split this aggregate category into 18 individual categories of solvent use. Beginning with Version 5 of the 1980 NAPAP inventory, emissions previously reported under Category 53 were disaggregated into these individual categories (78-95).

U.S. Department of Labor statistics on 1980 working hours (U.S. Department of Labor, 1981) were consulted to derive national-level seasonal and daily temporal variation for each of these emission categories. Monthly

data on total hours worked served as the basis for seasonal allocation factors. For most categories, seasonal allocation is approximately uniform. Data on overtime hours worked served as the basis for daily factors; the assumption was made that all overtime hours were worked on weekends, and that three times as much overtime was worked on Saturdays as on Sundays. The length of a working day (e.g., 7am-6pm) was used to generate hourly factors for each category. In general, most emissions were allocated uniformly during this period, with a smaller percentage (20-25 percent) divided throughout the remainder of the day.

Minor Point Sources (Categories 96-99)

These area source emissions categories were originally created for the 1980 NAPAP inventory to account for small point sources of SO_2, NO_x, and TSP. For Version 2 of the 1985 inventory, these categories were based on the following emissions criteria:

- All individual points with emissions of less than 5 TPY of each pollutant (SO_2, NO_x, VOC, TSP, and CO);
- All points at any plant found to emit less than 100 TPY of each pollutant (100 TPY plants are determined by summing emissions for all points excluding the less than 5 TPY points noted in the criterion above).

Categories 96-98 account for emissions from minor coal, oil, and gas combustion sources, respectively. The seasonal factors for these categories were derived from electric generation data contained in the EPRI Regional Systems (EPRI, 1981). The EPRI report presents monthly peak load data for each of the six EPRI regions. It is likely that these regional data were averaged nationwide to produce the national seasonal factor. The seasonal splits used in NAPAP are 27 percent winter, 23 percent spring, 27 percent summer, and 23 percent fall. The uniform daily pattern is based upon the assumption that utility activity is constant throughout the week. The hourly profile indicates that most activity takes place during normal working hours.

Category 99 includes combustion sources for fuels such as coke and process gas, evaporative emissions, and all process emissions. Owing to the diversity of source types within this category, the temporal pattern assigned reflected a general operating schedule of 52 weeks per year, 5 days per week, and 8 hours per day.

Miscellaneous VOC Categories (Categories 100-109)
(Added for the 1985 NAPAP inventory)

The 1985 NAPAP inventory provides county-level VOC emissions estimates for several categories which have not previously been included as area source categories. Some of these categories, such as Bakeries and Synthetic Fiber Manufacturing, were included to reconcile the difference between the total emissions reported in the *National Air Pollutant Emissions Estimates 1940-1984* (EPA, 1986), and the emissions already accounted for by the NEDS point source data files. The remaining categories such as Publicly-Owned

Treatment Works (POTWs) and hazardous waste Treatment, Storage, and Disposal Facilities (TSDFs) have been included due to the difficulty of measuring emissions from specific points within these categories (e.g., aeration basins).

To develop temporal profiles for these ten categories, operating schedule data for similar point source categories in the NAPAP inventory were analyzed. Operating data included seasonal throughput percentages, as well as hours per day and days per week of process operation. As a result, it was found that all but two of the new categories were best represented by uniform profiles. For the remaining two categories (101, 105), factors were derived from mean operating schedule data for similar categories in the point source file. The derived factors are as follows:

Category 101

Seasonal	percentages of 10, 25, 40, and 25 (for winter, spring, summer, fall, respectively);
Daily	uniform over weekdays;
Hourly	uniform from 7 a.m. to 5 p.m.

Category 105

Seasonal	percentages of 24, 24, 26, and 26 (for winter, spring, summer, fall, respectively);
Daily	uniform over weekdays and Saturdays;
Hourly	uniform from midnight to 5 p.m.

POINT SOURCE TEMPORAL ALLOCATION FACTORS

Temporal allocation of point source data is accomplished by one of two methods. In most cases, operating schedule data included in point-source data records served as the basis for point source factors. However, given the magnitude of emissions from electric utility sources, process-specific factors were developed to more accurately characterize these sources.

Operating Data-Derived Factors

Most NAPAP point source emission records contain operating schedule data which make possible the point-specific temporal allocation of emissions. These data consist of information on:

- Seasonal throughput percentages;
- Days/week of process operation; and
- Hours/day of process operation.

These operating data were used to temporally apportion point source data for which specific temporal factors were not developed.

Seasonal factors were taken directly from seasonal throughout percentages. Daily factors were derived from the number of days per week which a process operates. Factors were calculated according to the following schedule:

If the process operates x days/week	Emissions are allocated as follows
1	Saturdays only
2	Equally on Saturdays and Sundays
3-5	Equally on weekdays only
6	Equally on weekdays and Saturdays
7	Equally on all days of the week

Hourly factors are based on the number of hours per day which a process operates. Factors were developed using the following method:

If the process operates x hours/day	Emissions are allocated as follows
1-17	Zero for midnight to 7:00 a.m.; equally for x hours beginning with 7:00 a.m.; and zero for hours remaining before midnight.
> 17	Equally among 24 hours of the day.

Point Source Temporal Factors for Electric Utilities

Because of the importance of electric power plants to total U.S. emissions of SO_2 and NO_x, and because detailed data are available for these sources, special process-level (fuel and state specific) temporal factors were developed for utilities during the NAPAP effort. Factors were originally developed during the NECRMP study for power plants within the Northeast Corridor. In development of the NAPAP inventories, most of the NECRMP factors were retained, while some were replaced by new factors derived from additional data. For sources outside the NECRMP region, some factors were based on NECRMP figures; however, most were developed using other data sources.

Seasonal factors for the temporal distribution of point source emissions were developed on a fuel- and state-specific basis for facilities in the NECRMP study area, using information from the U.S. DOE's 1979 Energy Data Reports (U.S. Department of Energy, 1979). Outside the NECRMP region, uniform seasonal allocation factors were assigned.

Daily factors were developed at the national level from weekly load cycle listings in the EPRI Regional Systems (Electric Power Research Institute, 1981). These daily factors were calculated by normalizing the averages of the daily load statistics contained in the EPRI report. The factors, which were compiled on a season-specific basis, assume 75-76 percent of weekly emissions are produced on weekdays, 12-13 percent are produced on Saturdays, and the remainder are generated on Sundays.

Fuel- and state-specific weekday hourly patterns for utility operation were developed during the NECRMP effort (Sellars, et al., 1982). Profiles were derived from hourly power plant fuel-use data collected during the development of the SURE inventory (Klemm and Brennan, 1981). The SURE data base included hourly fuel-use data for approximately 300 power plants within the SURE region (the eastern portion of the United States). These data were collected for several study periods in 1977-1978 and included data for each season. Fuel- and season-specific fuel-use patterns were averaged by state, then normalized to generate the NECRMP hourly patterns. Since there were no hourly fuel-use data available for Rhode Island or Vermont, weekday factors were assigned from Connecticut and New Hampshire, respectively. Outside the Northeast Corridor, hourly factors for weekdays were developed by taking averages of the NECRMP values. Since no weekend hourly factors were developed during the NECRMP study, national Saturday and Sunday hourly profiles were developed from weekly load cycle listings in EPRI Regional Systems (Electric Power Research Institute, 1981). These were calculated by normalizing the averages of hourly load statistics.

QUALITY ASSURANCE AND FACTOR ENHANCEMENTS

Quality assurance and enhancement of the NAPAP temporal allocation factors is an ongoing process. As described above, the addition of new source categories for the 1985 area source inventory required the creation of corresponding factor profiles. Continuing work includes enhancing the accuracy of these and existing allocation factors by examining alternative data sources which may provide more representative temporal data. Efforts focus on sources which are significant contributors to acid precipitation precursors (e.g., electric utilities), and for which data are readily available.

Factor Normalization

During development of the 1985 NAPAP inventory, quality control checks of temporally allocated emissions revealed that inaccuracies sometimes resulted when reaggregation of point and area source emissions was attempted. These inaccuracies resulted from the fact that temporal factors themselves did not always sum to

unity according to the prescribed algorithms in the Introduction to this section. This in turn, was caused by rounding errors which were produced when factors were stored as 3-4 place values in computerized data files. To preserve annual emissions totals following temporal allocation, it was necessary to: (1) normalize the temporal factors; and (2) store the normalized factors more accurately in data files (as eight-byte values of computerized variables).

Other Studies

As described above, emissions from utility point sources outside the NECRMP study area were assigned a uniform seasonal profile in early versions of the NAPAP temporal allocation factor file. As a result, large amounts of SO_x and NO_x emissions were allocated according to these default factors. Efforts to improve point source temporal allocation in the 1985 NAPAP inventory included:

- using seasonal throughput percentages on plant-level records as the primary source of seasonal allocation data; uniform profiles were used secondarily, and
- incorporation of more accurate utility operating data.

Updates to seasonal factors for electric utility sources were made primarily on the basis of monthly plant-level fuel use data from DOE/EIA Form 759. These data were aggregated to form seasonal activity factors at the plant-fuel or state-fuel level (See Appendix D). Fuel-specific, state-level factors for utility boilers were also developed on the basis of unpublished computerized monthly reports from DOE/EIA titled "R080-Report on Consumption" from December 1984 to December 1985.

Hourly generation data from 58 TVA coal-fired boilers were evaluated to produce point-level seasonal, as well as daily and hourly, temporal factors. These profiles were added to the temporal allocation factor file and necessitated data processing modifications to accommodate point-level factor assignment.

All seasonal factors derived from these analyses were incorporated as seasonal throughput percentages on point source annual emission records.

TEMPORAL ALLOCATION FACTOR FILE FORMATS

Formats for area and point source temporal factor files are given in Tables 2-2 and 2-3. Both factor files are organized as data sets in the programming language of SAS.* All data are represented as 8-byte variables. The factors themselves (SEA-, DAY-, and HOUR-type variables) are decimal fractions. All other values are integers.

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* SAS is a registered trademark of the SAS Institute, Cary, NC.

TABLE 2-2. FORMAT OF SAS DATA SET CONTAINING TEMPORAL ALLOCATION FACTORS FOR 1985 AREA SOURCE EMISSIONS DATA

Variable name	SAS variable length (bytes)	Description
NUM_DAY	8	Temporal Scenario Code
STATE	8	AEROS State Code
COUNTY	8	AEROS County Code
SCC	8	Area Source Category Code
SEA	8	Seasonal Temporal Allocation Factor
DAY	8	Daily Temporal Allocation Factor
HOUR1-HOUR24	8	Hourly Temporal Allocation Factors

TABLE 2-3. FORMAT OF SAS DATA SET CONTAINING TEMPORAL ALLOCATION FACTORS FOR 1985 POINT SOURCE EMISSIONS DATA

Variable name	SAS variable length (bytes)	Description
NUM_DAY	8	Temporal Scenario Code
STATE	8	AEROS State Code
COUNTY	8	AEROS County Code
PLANT_ID	8	NEDS Plant Identifier
POINT_ID	8	NEDS Point Identifier
SCC	8	Source Classification Code
SEA1-SEA12	8	Seasonal Temporal Allocation Factors
DAY1-DAY12	8	Daily Temporal Allocation Factors
HOUR1-HOUR2888	8	Hourly Temporal Allocation Factors

The value of the variable NUM_DAY defines the day type of a given temporal scenario record. In all, there are 12 day types, which are defined in Table 2-4. For area sources, the allocation factor file contains 12 records per SCC—one for each day type. For point sources, all 12 scenarios are processed during a single computer run, and are thus accommodated by a single record. Hence, each record in the point source factor file contains 12 seasonal factors, 12 daily factors, and 288 (12 x 24) hourly factors; the variable NUM_DAY has a constant value of 12 for point source records.

Beginning with Version 2 of the 1985 inventory, plant and point identification codes were added to the point source temporal allocation factor file to accommodate the aforementioned point-level factors, where present.

TABLE 2-4. TEMPORAL ALLOCATION SCENARIO TYPES

Reference number (NUM_DAY)	Scenario
1	Winter weekday
2	Winter Saturday
3	Winter Sunday
4	Spring weekday
5	Spring Saturday
6	Spring Sunday
7	Summer weekday
8	Summer Saturday
9	Summer Sunday
10	Fall weekday
11	Fall Saturday
12	Fall Sunday

SECTION 3

SPATIAL ALLOCATION FACTORS

INTRODUCTION

Spatial allocation factors were developed for the NAPAP inventories to apportion area source emissions from counties to a series of grid cells as required for modeling applications. The NAPAP grid system covers the United States and Canada and extends from 50° to 125° west longitude and 25° to 60° north latitude. However, for the purpose of this section of the document, only spatial surrogates developed for U.S. area source categories are considered. Canadian spatial factors are discussed in Appendix B. Grid cells are 1/6° latitude by 1/4° longitude (or approximately 20 x 20 km). The actual size of a grid cell is a function of latitude and decreases to the north. Figure 3-1 illustrates the extent of the NAPAP grid. It should be noted that this figure depicts 2/3° latitude by 1° longitude grids for visual clarity.

A spatial allocation factor assigns a portion of an individual county's area source emissions to a specific grid cell. Since the actual subcounty distribution of area source emissions is usually not known, emissions are assumed to be distributed according to the known distribution of another quantity, i.e., a surrogate indicator. For example, in County A, the total housing count is 1,000 units and the housing count of County A within grid cell (1,1) is 200. The spatial fraction for housing in grid cell (1,1) for County A is 0.20. Therefore, 20 percent of County A's area source emissions spatially allocated by housing (e.g., residential fuel) would be allocated to grid cell (1,1). This methodology assumes area source emissions occur uniformally across the entire area of the grid cell.

The goal of the NAPAP spatial allocation factor development effort was to create as many surrogate values as possible for each county, allowing the user maximum flexibility in assigning county-level emissions to specific grid cells. These surrogates are used to estimate the subcounty distribution of area source emissions. Fourteen surrogate indicators were developed for use with the NAPAP inventory based on housing, population, and land-use data. The categories and sources of data are summarized in Table 3-1. For 1985 NAPAP application, 6 of the 14 surrogates are used for spatial allocation. Table 3-2 contains a listing of the spatial surrogates and their assignment to each area source category.

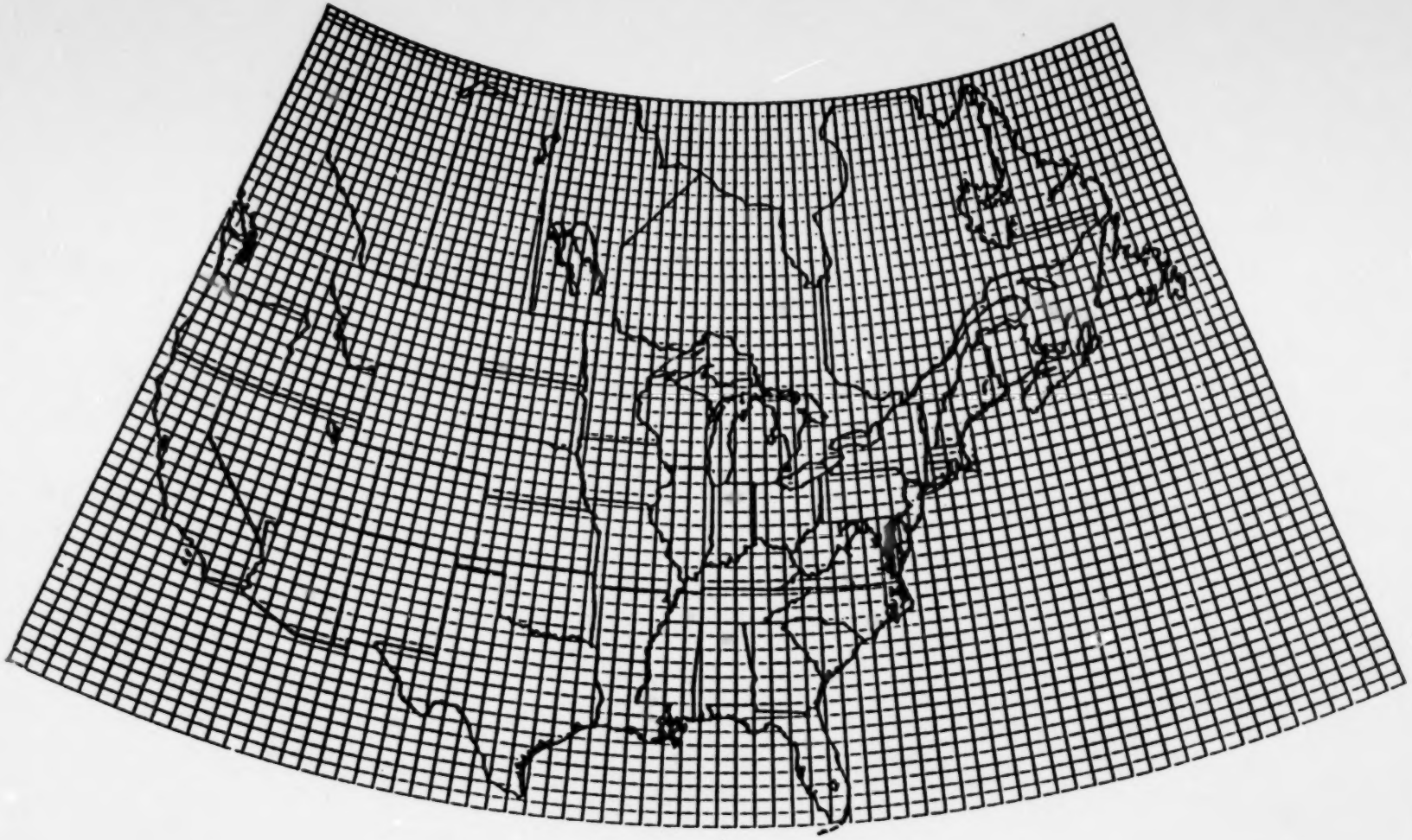

Figure 3-1. The extent of NAPAP grid. Note: 2/3° latitude by 1° longitude (approximate 80 x 80 km) grid cells are plotted in this figure.

Source: The Flexible Regional Emissions Data System for the 1980 NAPAP Emissions Inventory (Lebowitz and Ackerman. 1987).

TABLE 3-1. SPATIAL ALLOCATION SURROGATES AVAILABLE IN THE 1980 AND 1985 NAPAP SPATIAL ALLOCATION FACTOR FILES

Surrogate Indicator No.	Surrogate Indicator	Source
1	Population	1980 Census
2	Housing	1980 Census
3	Urban Land	Landsat
4	Agricultural Land	Landsat
5	Rangeland	Landsat
6	Deciduous Forest	Landsat
7	Coniferous Forest	Landsat
8	Mixed Forest and Forested Wetland	Landsat
9	Water	Landsat
10	Barren Land	Landsat
11	Nonforested Wetland	Landsat
12	Mixed Agricultural Land and Rangeland	Landsat
13	Composite Forest	Landsat
14	Land Area	EPA/Alliance

Note: The Landsat data are for 1972-1973.

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TABLE 3-2. SPATIAL ALLOCATION FACTOR SURROGATES FOR THE 1985 NAPAP AREA SOURCE EMISSIONS CATEGORIES

Category ID	Surrogate ID	Surrogate indicator	Emissions category
1	2	Housing	Residential Fuel--Anthracite Coal
2	2	Housing	Residential Fuel--Bituminous Coal
3	2	Housing	Residential Fuel--Distillate Oil
4	2	Housing	Residential Fuel--Residual Oil
5	2	Housing	Residential Fuel--Natural Gas
6	2	Housing	Residential Fuel--Wood
7	3	Urban Land	Commercial/Institutional Fuel--Anthracite Coal
8	3	Urban Land	Commercial/Institutional Fuel--Bituminous Coal
9	3	Urban Land	Commercial/Institutional Fuel--Distillate Oil
10	3	Urban Land	Commercial/Institutional Fuel--Residual Oil
11	3	Urban Land	Commercial/Institutional Fuel--Natural Gas
12	3	Urban Land	Commercial/Institutional Fuel--Wood
13	3	Urban Land	Industrial Fuel--Anthracite Coal
14	3	Urban Land	Industrial Fuel--Bituminous Coal
15	3	Urban Land	Industrial Fuel--Coke
16	3	Urban Land	Industrial Fuel--Distillate Oil
17	3	Urban Land	Industrial Fuel--Residual Oil
18	3	Urban Land	Industrial Fuel--Natural Gas
19	3	Urban Land	Industrial Fuel--Wood
20	3	Urban Land	Industrial Fuel--Process Gas
21	2	Housing	Incineration--Residential
22	3	Urban Land	Incineration--Industrial
23	3	Urban Land	Incineration--Commercial/Institutional
24	2	Housing	Open Burning--Residential
25	3	Urban Land	Open Burning--Industrial
26	3	Urban Land	Open Burning--Commercial/Institutional
27	14	Land Area	Light Duty Gas Vehicles--Limited Access
28	14	Land Area	Light Duty Gas Vehicles--Rural
29	2	Housing	Light Duty Gas Vehicles--Suburban
30	3	Urban Land	Light Duty Gas Vehicles--Urban
31	14	Land Area	Medium Duty Gas Vehicles--Limited Access
32	14	Land Area	Medium Duty Gas Vehicles--Rural
33	2	Housing	Medium Duty Gas Vehicles--Suburban
34	3	Urban Land	Medium Duty Gas Vehicles--Urban
35	14	Land Area	Heavy Duty Gas Vehicles--Limited Access
36	14	Land Area	Heavy Duty Gas Vehicles--Rural
37	2	Housing	Heavy Duty Gas Vehicles--Suburban
38	3	Urban Land	Heavy Duty Gas Vehicles--Urban
39	14	Land Area	Off-Highway Gas Vehicles
40	14	Land Area	Heavy Duty Diesel Vehicles--Limited Access
41	14	Land Area	Heavy Duty Diesel Vehicles--Rural
42	2	Housing	Heavy Duty Diesel Vehicles--Suburban
43	3	Urban Land	Heavy Duty Diesel Vehicles--Urban
44	14	Land Area	Off-Highway Diesel Vehicles
45	3	Urban Land	Railroad Locomotives
46	1	Population	Aircraft--Military

(continued)

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TABLE 3-2 (continued)

Category ID	Surrogate ID	Surrogate indicator	Emissions category
47	1	Population	Aircraft--Civil
48	1	Population	Aircraft--Commercial
49	1	Population	Vessels--Coal-Powered
50	1	Population	Vessels--Diesel
51	1	Population	Vessels--Residual Oil
52	1	Population	Vessels--Gasoline
54	1	Population	Gasoline Marketed
55	14	Land Area	Unpaved Roads
56	14	Land Area	Unpaved Airstrips
60	13	Composite Forest	Forest Wild Fires
61	13	Composite Forest	Managed Burning - Prescribed
62	4	Agricultural Land	Agricultural Field Burning
64	2	Housing	Structural Fires
66	14	Land Area	Ammonia Emissions--Light Duty Gasoline Vehicles
67	14	Land Area	Ammonia Emissions--Heavy Duty Gasoline Vehicles
68	14	Land Area	Ammonia Emissions--Heavy Duty Diesel Vehicles
69	4	Agricultural Land	Livestock Waste Management - Turkeys
70	4	Agricultural Land	Livestock Waste Management - Sheep
71	4	Agricultural Land	Livestock Waste Management - Beef Cattle
72	4	Agricultural Land	Livestock Waste Management - Dairy Cattle
73	4	Agricultural Land	Livestock Waste Management - Swine
74	4	Agricultural Land	Livestock Waste Management - Broilers
75	4	Agricultural Land	Livestock Waste Management - Other Chickens
76	4	Agricultural Land	Anhydrous NH3 Fertilizer Application
77	4	Agricultural Land	Beef Cattle Feed Lots
78	1	Population	Degreasing
79	1	Population	Drycleaning
80	1	Population	Graphic Arts/Printing
81	1	Population	Rubber and Plastic Manufacturing
82	1	Population	Architectural Coating
83	1	Population	Auto Body Repair
84	1	Population	Motor Vehicle Manufacturing
85	1	Population	Paper Coating
86	1	Population	Fabricated Metals
87	1	Population	Machinery Manufacturing
88	1	Population	Furniture Manufacturing
89	1	Population	Flat Wood Products
90	1	Population	Other Transportation Equipment Manufacturing
91	1	Population	Electrical Equipment Manufacturing
92	1	Population	Ship Building and Repair
93	1	Population	Miscellaneous Industrial Manufacturing
95	1	Population	Miscellaneous Solvent Use
96	1	Population	Minor Point Sources - Coal Combustion
97	1	Population	Minor Point Sources - Oil Combustion
98	1	Population	Minor Point Sources - Natural Gas Combustion
99	1	Population	Minor Point Sources - Process Sources
100	1	Population	Publicly Owned Treatment Works (POTWs)

(continued)

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TABLE 3-2 (continued)

Category ID	Surrogate ID	Surrogate indicator	Emissions category
101	14	Land Area	Cutback Asphalt Paving Operation
102	1	Population	Fugitives from Synthetic Organic Chemical Mfg.
103	1	Population	Bulk Terminal and Bulk Plants
104	1	Population	Fugitives from Petroleum Refinery Operations
105	1	Population	Process Emissions from Bakeries
106	1	Population	Process Emissions from Pharmaceutical Mfg.
107	1	Population	Process Emissions from Synthetic Fibers Mfg.
108	1	Population	Crude Oil and Natural Gas Production Fields
109	1	Population	Hazardous Waste Treatment, Storage, and Disposal Facilities (TSDFs)

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Once the subcounty distribution of each surrogate indicator was determined, area source emissions categories were matched to the spatial fractions corresponding to the most appropriate surrogate indicators. The resultant file, the Spatial Allocation Factor File (SAFF), is input to the Spatial Allocation Module (SAM) of the Flexible Regional Emissions Data System (FREDS) (Modica, et al, 1989) to spatially distribute area source emissions among 1/6° latitude by 1/4° longitude grid cells.

SPATIAL FACTOR DEVELOPMENT

The development of spatial allocation factors for the NAPAP effort (Beaulieu, et al., 1988) was based on two main sources of data: U.S. Department of Commerce, Bureau of the Census, Census of Population (POP) and Housing (HSG), 1980, and land use/classification data derived from 1972-1973 Landsat satellite imagery and land use/cover maps. Separate software was created to process each type of data into a format suitable for NAPAP applications. A simplified flow diagram of spatial factor processing is presented in Figure 3-2.

Population and housing data are processed through a series of three sequential computer programs. These programs, written in Fortran, are executed on the NCC Sperry UNIVAC. CREATE7A reads EPA's STF3A tape (census summary tape File 3A) for each state requested and writes a condensed census file. CREATE5A reads the condensed census file and a user-defined grid to generate subcounty gridded census data (e.g., population). For the State of Virginia, gridded census fractions are modified by the program VIRGINIA to avoid double counting or omission of the state's independent cities.

The land use spatial factor processing is accomplished by a Fortran program NEWLAND, executed on the NCC Sperry UNIVAC. Prior to NEWLAND, software developed by the Environmental Sciences Research Laboratory (ESRL) uses the NAPAP grid and county boundary definitions from the County Dime File to generate the county-grid relationships. These fractions are used by NEWLAND to reprocess the land use spatial fractions supplied as the percent land use of each grid cell to the fractional county land use for each grid cell. The resultant output file contains land use spatial fractions for 12 surrogates by state, county, column, and row.

Once spatial fractions are generated from the Census and Landsat data, the files are merged in SPACEMERGE to form a data set containing state, county, column, row, and 14 spatial surrogates (2 census and 12 land use surrogates) for each record. In addition, Massachusetts land use fractions, reported relative to county totals are modified relative to Air Pollution Control Districts using the Massachusetts adjustment data. Once the Census and Landsat data are merged, the data are converted to EBCDIC characters and transferred to the NCC's IBM 3090. For final processing, spatial fractions for land use and census surrogates are matched to area source categories in the Spatial Allocation Factor Preprocessor (SAFP) using a surrogate

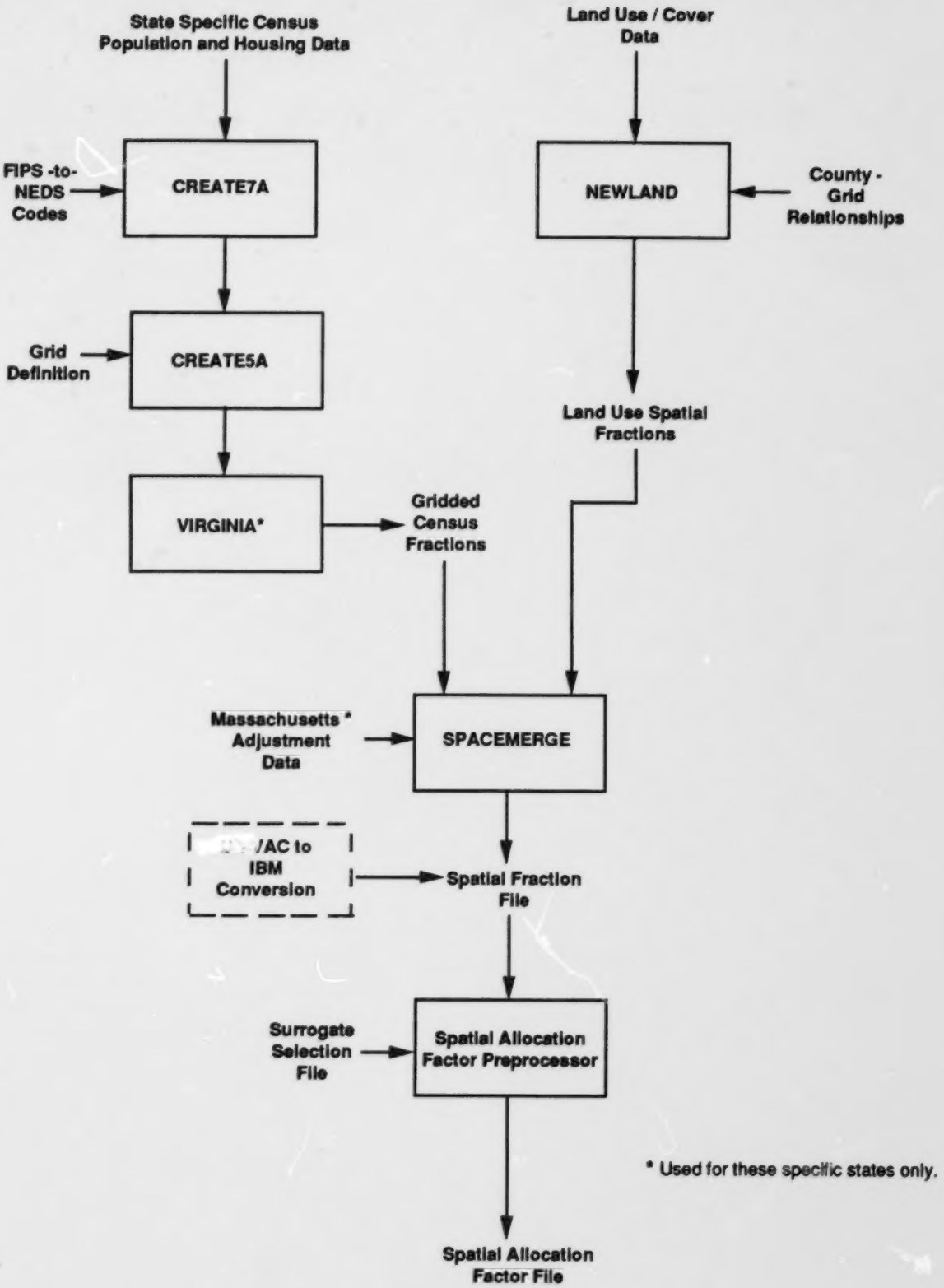

Figure 3-2. Simplified flow diagram of U.S. spatial factor processing.

selection file containing category number and the spatial surrogate assigned to each category. SAFP writes an EBCDIC file which is compatible with the Spatial Allocation Module of FREDS.

Spatial allocation factors for the 1985 NAPAP inventory are based on those developed for the 1980 effort. Quality control checks performed on the spatial factors and adjustments made to the factors for use with the 1985 NAPAP inventory are discussed in this section.

Grid Description

The grid system defined for U.S. spatial factor development is comprised of 37,440 grid cells (156 rows, 240 columns), each 1/6° latitude by 1/4° longitude (approximately 400 km²). Grid cell size is a function of latitude and varies in the United States from about 335 km² in Lake of the Wood County, Minnesota to 466 km² in Monroe County, Florida. The boundaries extend from 65° to 125° west longitude and from 25° to 51° north latitude. The cell at the southwestern corner of the grid is denoted (1,1), with column numbers increasing west to east, and rows from south to north. Column and row numbers are calculated from latitude and longitude as follows:

$$\text{column} = ((\text{WLNG} - \text{Longitude}) \times \text{DLON}) + 1 \quad (3.1)$$

$$\text{row} = ((\text{Latitude} - \text{SLAT}) \times \text{DLAT}) + 1 \quad (3.2)$$

where:

WLNG = Western boundary of the grid (125° for NAPAP)

DLON = The number of grids/degree longitude (4 for NAPAP)

SLAT = Southern boundary of the grid (25° for NAPAP)

DLAT = The number of grids/degree latitude (6 for NAPAP)

The resultant integer parts are the column and row numbers; fractional parts are truncated.

Population and Housing Factors

The starting point of the census-based spatial allocation surrogates is the U.S. Department of Commerce, Bureau of the Census, Census of Population and Housing, 1980. The file consists principally of sample data expanded to represent the total population. However, data pertinent to persons and housing units are based upon 100 percent counts and unweighted sample counts (U.S. Bureau of the Census, 1982).

Census data are summarized at the state (or state equivalent) level, and are broken down in hierarchical sequence, to the following levels: counties or county equivalents, minor civil divisions (MCDs) or census county divisions (CCDs), places or place segments within MCDs/CCDs and remainders of MCDs/CCDs, census tracts or block numbering areas (BNAs), and block groups (BGs) or, for areas that are not

block-numbered, enumeration districts (EDs). In addition, place and congressional districts (districts delineated for the 96th Congress) are presented separately from the hierarchical summary organization.

The longitude, latitude, and land area data fields in the state-specific census population and housing Summary Tape File 3A (STF3A) (U.S. Bureau of the Census, 1982) are blank. EPA inserted values for these fields using the Master Area Referenced File (MARF)2 (U.S. Bureau of the Census, 1983). The modified census tapes were used to generate the NAPAP spatial factors.

Generation of the housing and population-based spatial allocation factors involves executing three separate Fortran programs: CREATE7A, CREATE5A, and VIRGINIA. For Massachusetts, census-based spatial allocation factors are calculated relative to Air Pollution Control Districts (APCDs). (Massachusetts reports emissions data by APCD rather than at the county level). In the census data, independent cities are reported with the county level records for Virginia. Ten of the 41 independent cities are treated as county equivalents for NAPAP. These include Alexandria, Chesapeake, Fairfax, Hampton, Newport News, Norfolk, Portsmouth, Richmond, Suffolk, and Virginia Beach. The remaining 31 independent cities are merged into their respective counties (thus the need for the program VIRGINIA).

Land Use Spatial Factors

Development of the land use derived spatial allocation factors required two data files: land use/cover percentages for 1/6° latitude by 1/4° longitude grid cells and country-grid area relationships. The land use/cover data base was developed by Lockheed Engineering and Management Services Company's Remote Sensing Laboratory under contract for the Meteorology and Assessment Division of EPA's Environmental Sciences Research Laboratory (ESRL), currently Atmospheric Sciences Research Laboratory (ASRL). The data base was developed using Landsat mosaic images covering the periods July 23 to October 31, 1972 and January 1 to March 31, 1973, and from Land Use and Land Cover Maps developed in the middle-to-late 1970's. The development of the land use percentages has been previously summarized (Sellars, et al, 1985).

The total land use/cover in each grid cell is divided into the following classifications:

- Urban Land
- Agricultural Land
- Rangeland
- Deciduous Forest Land
- Coniferous Forest Land
- Mixed Forest Land (includes forested wetlands)
- Water
- Barren Land
- Nonforested Wetland
- Mixed Agricultural Land and Rangeland
- Rocky and open areas occupied by low growing shrubs and lichens

Each land classification percentage reported by Lockheed represents the portion of a grid cell comprised of a specific land use category. For NAPAP spatial factor processing, the category "Rocky and open area occupied by low growing shrubs and lichen" was not used. In addition to the eleven land use/cover categories supplied by Lockheed, two additional categories were calculated for NAPAP:

- Composite Forest
- Land Area

Composite Forest is comprised of coniferous, deciduous, and mixed forest lands for each grid cell (this summation is performed prior to the allocation of grid cells to counties). Land area is the fraction of a county's total land area contained within a grid cell and is calculated from data in the county-grid file discussed below.

Use of the land classification data for allocation of county-wide emissions totals to grid cells required that the gridded land use/cover data be summed to the county level. To allocate grid cells to counties, a data file containing county-grid relationships was created. The county-grid file was generated using a file containing county boundaries (the County Dime File) in conjunction with the NAPAP grid system and software developed by ESRL. County-grid relationships were calculated as the fraction of each county in each grid cell. These relationships were used to aggregate the grid-level land use data to the county-level such that county-level allocation factors could be determined. An example of this process is illustrated in Figure 3-3.

Applying the county-grid file to the land use/cover percentages allows gridded land use fractions to be expressed as the fraction of a county's land use/cover in a grid cell. Spatial allocation factors for each land use classification are calculated as follows:

$$SAF_{cxi} = \frac{(A_{ci})\,(A_{xi})}{\sum_{i=1}^{n} (A_{ci})\,(A_{xi})}$$

where: SAF_{cxi} = The spatial allocation factor for County C, land use type X, and grid i.

A_{ci} = The portion of County C that falls within grid i.

A_{xi} = The portion of grid i with land use type X.

n = The number of grids covering County C.

The fractional totals for each county sum to 1; fractional totals by grid cell do not sum to a particular number. The land use and county-grid fractions are processed by the program NEWLAND.

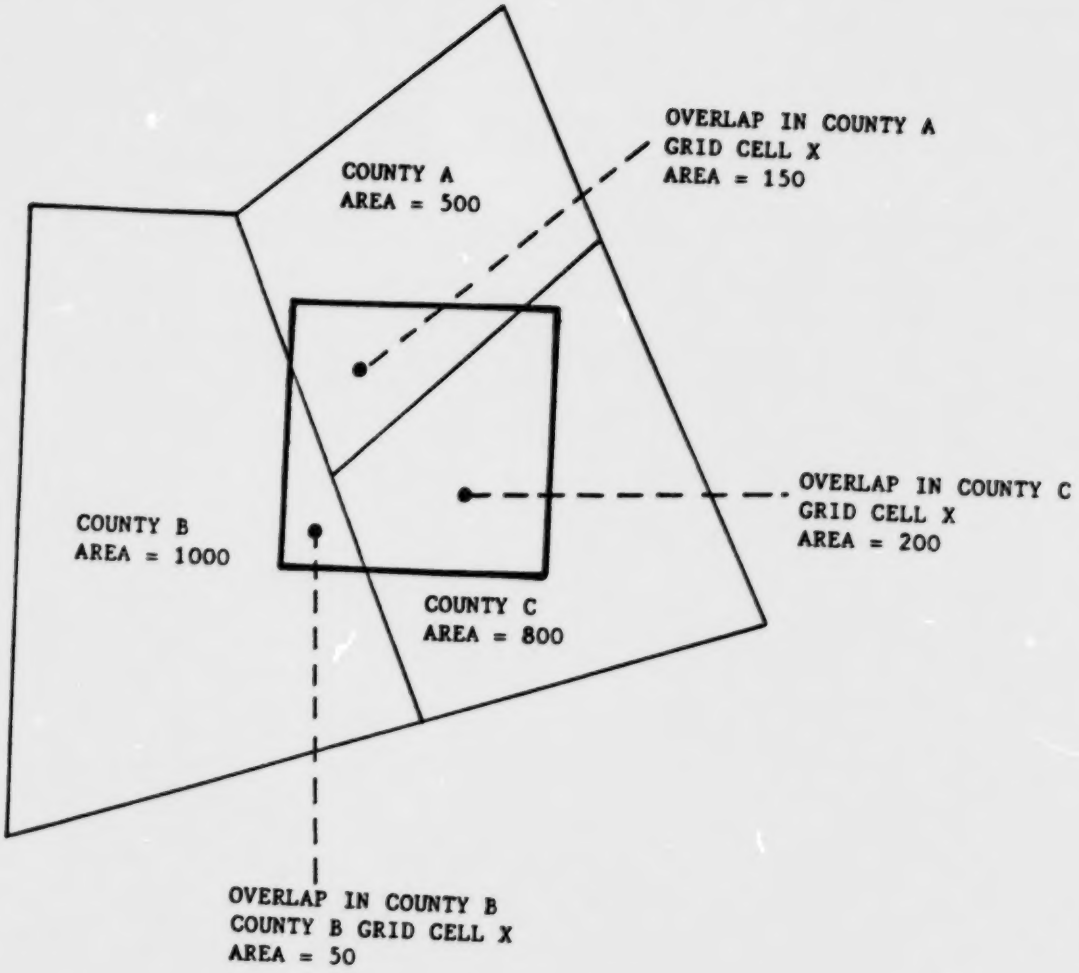

Figure 3-3. Example of county-to-grid cell areal relationship.

Source: National Acid Precipitation Assessment Program Emission Inventory Allocation Factors (Sellars et al., 1985).

QUALITY CONTROL AND ENHANCEMENTS OF SPATIAL FACTORS FOR THE 1985 NAPAP INVENTORY

Spatial allocation factors were originally developed for processing the 1980 NAPAP area source inventory. To assure the quality of the spatially resolved 1985 area-source emissions, extensive quality control checks were performed on spatial factors adopted from the previous NAPAP data base. The goal of the spatial factor quality control procedures was to ensure complete and accurate apportionment of NAPAP area source emissions. Based on the results of these checks, adjustments were made to the spatial fractions for use with the 1985 NAPAP inventory. Additional modifications to the file were required for spatial allocation of emissions from the new 1985 NAPAP area source categories and Cibola County, New Mexico. Quality Control procedures and modifications made to the Spatial Allocation factors are discussed below and in Appendix A.

Quality Control Procedures

Quality control procedures for the spatial allocation factors fell into three general categories: evaluation of emissions losses during inventory processing in the Spatial Allocation Module (SAM) (based on the Quality Control Module (QCM) processing messages); analyses of counties requiring normalization for spatial surrogates deviating by 20 percent or more as noted in the Spatial Allocation Factor Preprocessor (SAFP) processing messages; and "other analyses" including a review of the spatial factor computer programs and the Massachusetts county-to-APCD conversion.

The causes of the emissions losses during inventory processing were evaluated by comparing county- and SCC-level emissions totals before and after spatial allocation, matching state/county codes in the emissions file with those in the Spatial Allocation Factor File (SAFF), and tracking specific counties through various stages of the spatial factor processing. Counties and surrogates identified by the SAFP processing messages as requiring excessive normalization were analyzed using grid maps for each state, atlases, and data from various segments of the spatial factor development process. In addition, segmented maps were plotted as necessary and included the locations of various towns for reference. Location data for these maps were obtained from the National Cartographic Information Center. Other quality control procedures included close examination of the spatial software and applications of these programs for other projects.

Quality control checks applied to the 1980 NAPAP spatial allocation factors revealed several problems with the data. These are summarized in Table 3-3 and are discussed in greater detail in Appendix A.

Adjustments to Spatial Allocation Factors

For 1985 NAPAP applications, adjustments were made to the 1980 spatial fractions to account for missing and new counties, missing grid cells, incorrect county code assignments and location data, inaccuracies in the

TABLE 3-3. SUMMARY OF 1980 SPATIAL FACTOR PROBLEMS AND IMPACTS[a]

Problem	Areas Affected	Reason	Impacts
Missing Counties			
1. From Land Use File	Sabine, LA; Barbour, WV	Unknown - Present in CNTY2GRID[b] File	Loss of emissions
	Alexandria, VA; Chesapeake, VA; Fairfax, VA; Portsmouth, VA; Richmond, VA	Some Virginia independent cities were incorrectly coded in CNTY2GRID[b] File	Loss of emissions
	Menominee, WI	Menominee is an Indian reservation within Shawno County. For Census processing, Menominee was assigned the county code for Shawno	Loss of emissions
2. From FIPAEROS File[c]	Nansemond, VA	Instead of assigning Suffolk independent city to Nansemond County, the code for Suffolk was used	Loss of emissions
3. New County	Cibola, NM	Separated from Valencia County in 1982; not a county for 1980	Loss of emissions
Missing Grid Cells			
1. From Land Use File	Alexander, IL; Queen Annes, MD; Dare, NC	Grid cells not in CNTY2GRID[b] File	Incorrect Census fractions (off by 20% or more before normalization)
	Monroe, FL	Some segments below NAPAP southern boundary; the remainder is unknown	Incorrect Census fractions (off by 20% or more before normalization)
County Code Assignments			
1. FIPAEROS File[c]	Saginaw, MI	Input as two county codes - 4600 and 4780 in land use; 4600 only in Census data. County 4600 does not exist so emissions are matched to 4780 which shows no Census fractions	Incorrect Census fractions (off by 20% or more before normalization)

(continued)

TABLE 3-3 (continued)

Problem	Areas Affected	Reason	Impacts
	Jackson, SD; Washabaugh, SD	Treated as separate counties in land use and emissions files, but as single county in Census data (for certain applications, these are treated as a single county)	Incorrect Census fractions (off by 20% or more before normalization)
2. Land Use File	Lincoln, OR; Linn, OR	These were interchanged in the land use file - grids belonging to Lincoln were assigned to Linn and vice versa	Incorrect Census fractions (off by 20% or more before normalization)
Location Data			
1. Census File	Rappahannock, VA	Grid cell located outside county	Incorrect Census fractions (off by 20% or more before normalization)
	Adams, WI	Latitude/longitude of county and subcounty centroids do not correspond to Adams County grid cells	Incorrect Census fractions (off by 20% or more before normalization)
2. Independent city assigned to county which it is not within geographically	Pulaski, VA	Unknown	Incorrect Census fractions (off by 20% or more before normalization)
Massachusetts County to APCD Conversion			
1. County to APCD Area Adjustment	Berkshire, Central Massachusetts, Merrimack Valley, Metropolitan Boston, Pioneer Valley, and Southeastern Massachusetts APCDs	County to APCD area conversion was not done in SPACEMERGE; Border grid cells assigned to only <u>one</u> grid cell based on a value of population rather than area	Spatial distribution of emissions not accurately represented
Algorithms			
1. CREATE5A column and row equations	Border grid cells when a subset of the NAPAP grid is specified (incorrect coordinates)	Equation does not account for a subset of the NAPAP grid	Does not impact NAPAP

(continued)

TABLE 3-3 (continued)

Problem	Areas Affected	Reason	Impacts
2. SPACEMERGE grid to column and row equations	Eastern border grids	Equation does not correctly deal with the eastern boundary of the grid	Land use data in the eastern boundary is shifted one cell to the north; the COL equation yields a column number of 0 instead of 240
3. SAFP Normalization	County totals off by less than 5%	Algorithm only checks for county/surrogate totals off by 5% or more; normalization algorithm doesn't allow county to sum exactly to 100% (approaches it, but never reaches it)	Minor loss of emissions (<0.1%)
4. SAFP Combination	Massachusetts	Equation did not combine each succeeding state, county, col, row combination which matched the previous record. Instead it added the spatial fractions from the first similar record to itself	Spatial distribution of emissions not accurately represented

[a]More complete discussions of spatial factor problems and adjustments are presented in Appendix A.

[b]Contains county-to-grid fractions

[c]Contains FIPS to NEDS code conversions

Massachusetts county-to-APCD conversion and the new area source categories. All corrections were applied to the SAFP input file (the spatial fraction file) and are summarized in Table 3-4. Once adjustments were made to the spatial fraction file, SAFP was executed and the processing messages were evaluated to assure the factors were correctly applied. Corrections and enhancements to the spatial fractions are also summarized in Appendix A.

SPATIAL ALLOCATION FACTOR FILE FORMAT

The Spatial Allocation Factor File is an EBCDIC file containing one record type. Each record contains all of the spatial allocation information for a particular SCC in a specific county. The detailed format is contained in Table 3-5.

TABLE 3-4. SUMMARY OF SPATIAL FACTOR ADJUSTMENTS FOR THE 1985 NAPAP INVENTORY*

Problem	Areas affected	Adjustments
Missing counties	Alexandria, VA; Chesapeake, VA; Fairfax, VA; Nansemond, VA; Portsmouth, VA; Richmond, VA; Barbour, WV	Population and housing fractions available from a previous project.
	Cibola, NM	Adjust population, housing, and total land area fractions for Valencia to account for new county boundary.
	Sabine, LA; Menominee, WI	Calculate land area fractions and insert into population field.
Missing grid cells	Queen Annes, MD	Population and housing fractions available from a previous project.
	Alexander, IL	Insert missing population and housing fraction into single missing grid cell.
	Monroe, FL; Dare, NC	Calculate population fractions for missing grid cells from town populations and latitude/longitude data.
County code assignments	Saginaw, MI	Verify correct county code and adjust in spatial fraction file.
	Lincoln, OR; Linn, OR; Jackson, SD; Washabaugh, SD	Insert land area fractions into the population field; zero out housing values.
Location data	Pulaski, VA	Normalize in SAFP.
	Rappahannock, VA	Assign missing population and housing fractions to appropriate grid cell.
	Adams, WI	Substitute land area fractions in population field.
Massachusetts county to APCD conversion	Berkshire, Central Massachusetts, Merrimack Valley, Metropolitan Boston, Pioneer Valley, and Southeastern Massachusetts	Calculate new land area fractions; zero out all other land use spatial fraction fields.
Algorithms		Modify all problematic algorithms for future processing.

*A more complete discussion of spatial factor adjustments and enhancements is presented in Appendix A.

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TABLE 3-5. FILE FORMAT FOR THE EBCDIC 1985 SPATIAL ALLOCATION FILE

Record position		Column width	Format	Variable name	Description
First	Last				
1	2	2	I	STATE	AEROS State Code
3	6	4	I	COUNTY	AEROS County Code
7	9	3	I	SCC	Area Source Category Code
10	12	3	I	NGRID	Number of Grids in County
13	16	4	I	NROW	Row of Grid Cell
17	20	4	I	NCOL	Column of Grid Cell
21	25	5	F5.4	NSAF[a]	Spatial Allocation Factor for Grid Cell[b]

[a]Implied decimal, with four digits to the right of the decimal place and one to the left.

[b]Spatial allocation factors are dimensionless fractions representing the portion of a county's land use for a specific land use category in a grid cell.

Note: Columns 13 to 25 are repeated up to NGRID times.

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SECTION 4

SPECIES ALLOCATION FACTORS

INTRODUCTION

One of the primary end uses of the 1985 NAPAP inventory is as input to models such as the Regional Acid Deposition Model (RADM). RADM includes a chemical reaction mechanism to simulate the transformation of primary emissions into stable product species during atmospheric transport. Certain pollutants in the NAPAP annual inventory represent composites of various reported compounds in an aggregated format too general to be useful as input to the model. As a result, three pollutants - total hydrocarbons (THC), oxides of nitrogen (NO_x), and total suspended particulates (TSP) - must be resolved into component species or groups of species which share similar reaction chemistry prior to RADM input. Specifically, the NAPAP modeler's inventory includes NO and NO_2, 32 classes of hydrocarbon species, and 15 particulate fractions based on alkalinity and size distribution.

The allocation of pollutants to species classes is accomplished using speciation profiles, which provide a breakdown of THC, TSP, and NO_x emissions to a typical set of component classes. The profiles are generally process-specific, and are matched with emissions records at the level of point source SCC or NEDS/NAPAP area source category.

The earliest speciation efforts, using the Regional Model Data Handling System (RMDHS), could accommodate only ten hydrocarbon classes and no particulate speciation was attempted. With the development of the Flexible Regional Emissions Data System, a significant increase in the number of allowable speciated components was achieved. The final version of the base year 1980 inventory contained 28 hydrocarbon species, as well as a preliminary allocation of particulate matter into four alkalinity classes.

In support of the expanded RADM requirements for the 1985 inventory, and the increasing need for representative speciation data for numerous EPA research efforts, Radian Corporation performed a comprehensive review and update of existing hydrocarbon and particulate speciation data (Shareef, et al., 1988). These data were reviewed by Alliance and subsequently manipulated into a format consistent with NAPAP inventory processing needs. In addition, extensive modifications to FREDS were undertaken to accommodate an increased number and expanded format for the 1985 species classes.

The remainder of this section describes in detail the development of the speciation factors used in the 1985 NAPAP modeling inventory, including sources of data, quality assurance, and procedures used to convert data to a format suitable for NAPAP. Also included is a section describing the preprocessing of hydrocarbon emissions using data from the speciation files.

HYDROCARBON/NOx SPECIATION FACTOR DEVELOPMENT

Methodology

Regional models such as RADM employ algorithms to simulate the complex transformation processes occurring in the atmosphere. These reaction mechanisms are applied to classes of organic compounds, each of which may include a number of individual species with similar reaction properties and reaction products. For example, several C4 through C6 olefine may be satisfactorily expressed by a single set of reaction statements and, therefore, be represented by a single species class in the model. The RADM species classes used in the 1985 NAPAP modeling inventory are depicted in Table 4-1.

Since early in the NAPAP inventory development effort, it has been recognized that flexibility in speciation is desirable to accommodate the needs of different modeling chemistries. Speciated VOC data are also required for other EPA activities including ozone and air toxics studies. Therefore, hydrocarbon species data are coded as a set of species profiles, each of which provides a breakdown of the representative component species for a source's hydrocarbon emissions. The profiles can then be manipulated by the end user to represent any desired classification scheme.

For the NAPAP inventory, species profiles and class assignments are used to create speciation factors for hydrocarbons by means of a computer program called the Pollutant Splits System (PSPLIT). PSPLIT is a Fortran program that can divide hydrocarbon emissions into over 600 discrete species based on Source Classification Code (SCC) specific profiles. The individual species are subsequently reaggregated into up to 32 classes based on the requirements of the selected transport model.

Three data files are required as input to PSPLIT. The Species-Profile file contains the weight percent contribution of each species to each profile. Each individual species is assigned to a reactivity class in the Species-Class file. Finally, profiles are matched to NAPAP emissions records using the SCC-Profile Index file. PSPLIT performs the appropriate processing steps to calculate the amount of total hydrocarbon that contributes to each class, for every source category in the inventory. The resulting mole factors are expressed in moles/kilogram and when multiplied by the mass of total hydrocarbon from a source, they yield the number of moles of each class emitted.

TABLE 4-1. HYDROCARBON SPECIES CLASSES, 1985 NAPAP RESOLVED INVENTORY

Class number	Description
1	Methane
2	Ethane
3	Propane
4	Alkanes (0.25 - 0.50 reactive)*
5	Alkanes (0.50 - 1.00 reactive)
6	Alkanes (1.00 - 2.00 reactive)
7	Alkanes (> 2.00 reactive)
8	Alkane/aromatic mix
9	Ethene
10	Propene
11	Alkenes (primary)
12	Alkenes (internal)
13	Alkenes (primary/internal mix)
14	Benzene, halobenzenes
15	Aromatics (< 2.00 reactive)
16	Aromatics (> 2.00 reactive)
17	Phenols and cresols
18	Styrenes
19	Formaldehyde
20	Higher aldehydes
21	Acetone
22	Higher ketones
23	Organic acids
24	Acetylene
25	Haloalkenes
26	Unreactive
27	Others (< 0.25 reactive)
28	Others (0.25 - 0.50 reactive)
29	Others (0.50 - 1.00 reactive)
30	Others (> 1.00 reactive)
31	Unidentified
32	Unassigned

*Reactivity is defined with respect to rate constant range (with OH), 10^4 ppm^{-1} min^{-1}.

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PSPLIT is also used to disaggregate NO_x emissions into NO and NO_2 components. The species profiles input to PSPLIT contain the weight fractions of NO and NO_2, which are carried through the program and become the speciation factors for these two components.

Speciation File Development

The source of the hydrocarbon species profiles used in the 1985 NAPAP inventory is Radian Corporation's updated *Air Emissions Species Manual (Shareef, et al., 1988).* This document is largely based on the *Volatile Organic Compound (VOC) Species Data Manual - Second Edition* (EPA, 1980), which in turn formed the basis for earlier NAPAP speciation data gathering efforts. Revisions to the 1980 VOC Data Manual consisted of identifying and replacing poor quality and/or outdated profiles, and adding profiles to fill data gaps primarily in the area of air toxics.

New profiles were developed as a result of a literature search. Key sources of information included: a study conducted for the California Air Resources Board; source assessment and background information documents; Section 114 responses and trip reports from standard development activities; and work conducted by the Atmospheric Research and Exposure Assessment Laboratory (AREAL). Data from the Northeast Corridor Regional Modeling Project (NECRMP), current and past NAPAP work, Environment Canada, and State agencies were also reviewed. The effort resulted in the addition of nearly 200 new profiles, 80 percent of which covered source categories not characterized in the 1980 manual. An additional five profiles were developed from a speciation test program to characterize high priority emission sources. These profiles represent the following source categories: gasoline marketed, degreasing, dry cleaning, auto body repair, and graphic arts/printing.

In addition to profile development, Radian assigned each NEDS point source SCC and area source category to a hydrocarbon profile. Ideally, a separate profile would be needed to represent each category. However, the number of categories is significantly larger than the number of available profiles. Source categories without original profile assignments were, therefore, assigned to existing profiles using engineering judgement. In addition, 43 industry-specific average profiles were developed and applied to source categories for which a satisfactory assignment based on engineering judgement was not possible. Finally, for those sources not expected to report hydrocarbon emissions, a "zero" profile was generated; this profile is an overall average based on all the other profiles in the data base. The zero profile was intended for use only with SCCs characterized by "zero" or "negligible" VOC emission factors for which a State or other agency may have reported nonzero emissions.

The assignment of the nearly 650 individual hydrocarbon species to classes consistent with RADM chemistry was a collaborative effort coordinated by the National Center for Atmospheric Research (NCAR) representing NAPAP Task Group III (Atmospheric Transport and Modeling). Species classification was an iterative

procedure involving a number of individuals from the modeling community. During the process, the number of classes desired increased considerably in an attempt to accommodate as many different mechanisms as possible. Constraints on the number of classes which could be processed through NAPAP software limited the final class total to 32, although a 50-category scheme was also proposed. The NCAR classification scheme is to be used both for RADM and the Acid Deposition and Oxidant Model (ADOM); a separate classification mechanism based on carbon bond classes is being developed for the Regional Oxidant Modeling for Northeast Transport (ROMNET) program.

NO_x speciation fractions represent NO and NO_2 fractions recommended by AP-42 (EPA, 1985), and were adapted from the 1980 data with little modification. In previous applications, profiles that were applied to an SCC that was not expected to have NO_x emissions were assigned profile splits of zero for both NO and NO_2. It was of concern that NO_x emissions could be lost during the FREDS speciation step if a source with NO_x emissions was misassigned to an SCC that was represented by zero splits for NO and NO_2. To ensure that no NO_x emissions are lost, a default split of 95 percent NO and 5 percent NO_2 was substituted for every profile which did not have an explicit NO/NO_2 split.

Quality Control Checking

Prior to PSPLIT execution, the three component speciation files were subjected to a quality control review involving manual and automated data checks. These screening checks were designed primarily to detect missing, invalid, duplicate, or inconsistent data elements within the computer files. No attempt was made to verify the quality of the data upon which the speciation files were based. All findings were reported to Radian for review and correction.

One of the Radian profiles, corresponding to diesel vehicle exhaust emissions, was identified as too general for use in the NAPAP speciation methodology. The profile was based on analyses of diesel fuels and included species identified sequentially as "C2 compounds" through "C43 compounds". Neither the structure nor the chemical makeup of these 42 species were provided, and assignment to RADM classes was therefore not possible. The profile for diesel vehicle exhaust emissions developed for the 1980 inventory was modified based on information supplied by EPA (Black, F. personal communication with M. Saegar, Alliance), and used as a substitute for the 1985 inventory application.

The original 1980 profile was modified by adding the species o-xylene to represent the appropriate weight percent of high carbon number aromatics in diesel exhaust. The weight percent of n-pentadecane in the profile was decreased by the weight percent assigned to o-xylene.

A total of five area source categories (66 through 70) added late in the 1985 annual inventory development were not assigned to profiles by Radian. NAPAP data processing software requires that all source categories be assigned to profiles regardless of whether or not the category is likely to include hydrocarbon emissions. Therefore, the vehicular source ammonia categories (66, 67, and 68) and the new livestock waste management ammonia categories (69 and 70) were all assigned to the global default (0) hydrocarbon species profile.

The data processing requirements of the 1985 inventory made it necessary to revise the original PSPLIT computer code. This effort resulted in the creation of a new version of the program designated PSPLIT_2A. The new version differs from earlier versions as follows:

- The maximum allowable number of species per profile was increased from 75 to 325;
- The maximum allowable number of species in all classes was increased from 500 to 640;
- The maximum allowable number of SCC - Profile index records was increased from 1,800 to 4,000;
- The maximum allowable number of profiles was increased from 175 to 320;
- The maximum allowable number of species-level profile records was increased from 2,000 to 4,500; and
- The maximum allowable number of species classes was increased from 30 to 32.

In addition, the format of the output speciation factors was increased from four digits to five digits to increase the precision of species emission estimates.

FREDS Input File Format

The output of PSPLIT_2A for the RADM modeling inventory (known simply as the PSPLIT File) contains mole factors for the 32 hydrocarbon classes and weight percents for NO and NO_2 for each point and area source category in the annual file. The file is formatted as illustrated in Table 4-2, allowing it to be read by the FREDS Speciation Module. The file header information (record type 1) occupies the first two lines and contains codes which correspond to each of the 32 classes, 16 per line. The remainder of the file consists of a series of two-line speciation records (type 2), with 16 hydrocarbon speciation factors per line.

PARTICULATE SPECIATION FACTOR DEVELOPMENT

Methodology

Speciation factors for pollutants not handled by PSPLIT can be input to FREDS using an independent Speciation Factor File (SFF). For the 1985 modeling inventory, the SFF contains factors for 15 subspecies of particulate matter. Since particle size is an important criterion in TSP transport mechanisms, particulates are

TABLE 4-2. PSPLIT FILE FORMAT

Record position		Column width	Format	Variable name	Description
First	Last				
Header Record No. 1					
1	5	5	I	CLASS1	Pseudo-SAROAD code for THC Class No. 1
6	10	5	I	CLASS2	Pseudo-SAROAD code for THC Class No. 2
11	15	5	I	CLASS3	Pseudo-SAROAD code for THC Class No. 3
16	20	5	I	CLASS4	Pseudo-SAROAD code for THC Class No. 4
21	25	5	I	CLASS5	Pseudo-SAROAD code for THC Class No. 5
26	30	5	I	CLASS6	Pseudo-SAROAD code for THC Class No. 6
31	35	5	I	CLASS7	Pseudo-SAROAD code for THC Class No. 7
36	40	5	I	CLASS8	Pseudo-SAROAD code for THC Class No. 8
41	45	5	I	CLASS9	Pseudo-SAROAD code for THC Class No. 9
46	50	5	I	CLASS10	Pseudo-SAROAD code for THC Class No. 10
51	55	5	I	CLASS11	Pseudo-SAROAD code for THC Class No. 11
56	60	5	I	CLASS12	Pseudo-SAROAD code for THC Class No. 12
61	65	5	I	CLASS13	Pseudo-SAROAD code for THC Class No. 13
66	70	5	I	CLASS14	Pseudo-SAROAD code for THC Class No. 14
71	75	5	I	CLASS15	Pseudo-SAROAD code for THC Class No. 15
76	80	5	I	CLASS16	Pseudo-SAROAD code for THC Class No. 16
81	113	33	-	–	Unused
114	115	2	I	TYPE	Record Type (=11)
Header Record No. 2					
1	5	5	I	CLASS17	Pseudo-SAROAD code for THC Class No. 17
6	10	5	I	CLASS18	Pseudo-SAROAD code for THC Class No. 18
11	15	5	I	CLASS19	Pseudo-SAROAD code for THC Class No. 19
16	20	5	I	CLASS20	Pseudo-SAROAD code for THC Class No. 20
21	25	5	I	CLASS21	Pseudo-SAROAD code for THC Class No. 21
26	30	5	I	CLASS22	Pseudo-SAROAD code for THC Class No. 22
31	35	5	I	CLASS23	Pseudo-SAROAD code for THC Class No. 23
36	40	5	I	CLASS24	Pseudo-SAROAD code for THC Class No. 24
41	45	5	I	CLASS25	Pseudo-SAROAD code for THC Class No. 25
46	50	5	I	CLASS26	Pseudo-SAROAD code for THC Class No. 26
51	55	5	I	CLASS27	Pseudo-SAROAD code for THC Class No. 27
56	60	5	I	CLASS28	Pseudo-SAROAD code for THC Class No. 28
61	65	5	I	CLASS29	Pseudo-SAROAD code for THC Class No. 29
66	70	5	I	CLASS30	Pseudo-SAROAD code for THC Class No. 30
71	75	5	I	CLASS31	Pseudo-SAROAD code for THC Class No. 31
76	80	5	I	CLASS32	Pseudo-SAROAD code for THC Class No. 32
81	113	33	-	–	Unused
114	115	2	I	TYPE	Record Type (=12)

(continued)

TABLE 4-2 (continued)

Record position		Column width	Format	Variable name	Description
First	Last				
Speciation Record No. 1					
1	2	2	I	STATE	AEROS State Code
3	6	4	I	COUNTY	AEROS County Code
7	10	4	A	PLANT_ID	Plant Identification Code[a]
11	13	3	A	POINT_ID	Point Identification Code[a]
14	21	8	I	SCC	Area Source Category or Point Source SCC
22	26	5	F5V3[b]	TSF1	Speciation Factor, THC Class 1[c]
27	31	5	F5V3	TSF2	Speciation Factor, THC Class 2[c]
32	36	5	F5V3	TSF3	Speciation Factor, THC Class 3[c]
37	41	5	F5V3	TSF4	Speciation Factor, THC Class 4[c]
42	46	5	F5V3	TSF5	Speciation Factor, THC Class 5[c]
47	51	5	F5V3	TSF6	Speciation Factor, THC Class 6[c]
52	56	5	F5V3	TSF7	Speciation Factor, THC Class 7[c]
57	61	5	F5V3	TSF8	Speciation Factor, THC Class 8[c]
62	66	5	F5V3	TSF9	Speciation Factor, THC Class 9[c]
67	71	5	F5V3	TSF10	Speciation Factor, THC Class 10[c]
72	76	5	F5V3	TSF11	Speciation Factor, THC Class 11[c]
77	81	5	F5V3	TSF12	Speciation Factor, THC Class 12[c]
82	86	5	F5V3	TSF13	Speciation Factor, THC Class 13[c]
87	91	5	F5V3	TSF14	Speciation Factor, THC Class 14[c]
92	96	5	F5V3	TSF15	Speciation Factor, THC Class 15[c]
97	101	5	F5V3	TSF16	Speciation Factor, THC Class 16[c]
102	105	4	F4V4	HCHOWT	Weight Fraction Formaldehyde in Profile (dimensionless)
106	109	4	F4V3	TSF33	Speciation Factor for NO_2 (dimensionless weight fraction)
110	113	4	F4V3	TSF34	Speciation Factor for NO_2 (dimensionless weight fraction)
114	115	2	I	TYPE	Record Type (=21)
Speciation Record No. 2					
1	2	2	I	STATE	AEROS State Code
3	6	4	I	COUNTY	AEROS County Code
7	10	4	A	PLANT_ID	Plant Identification Code[a]
11	13	3	A	POINT_ID	Point Identification Code[a]
14	21	8	I	SCC	Area Source Category or Point Source SCC
22	26	5	F5V3[b]	TSF17	Speciation Factor, THC Class 17[c]
27	31	5	F5V3	TSF18	Speciation Factor, THC Class 18[c]
32	36	5	F5V3	TSF19	Speciation Factor, THC Class 19[c]
37	41	5	F5V3	TSF20	Speciation Factor, THC Class 20[c]
42	46	5	F5V3	TSF21	Speciation Factor, THC Class 21[c]
47	51	5	F5V3	TSF22	Speciation Factor, THC Class 22[c]
52	56	5	F5V3	TSF23	Speciation Factor, THC Class 23[c]

(continued)

TABLE 4-2 (continued)

Record position		Column width	Format	Variable name	Description
First	Last				
57	61	5	F5V3	TSF24	Speciation Factor, THC Class 24[a]
62	66	5	F5V3	TSF25	Speciation Factor, THC Class 25[a]
67	71	5	F5V3	TSF26	Speciation Factor, THC Class 26[a]
72	76	5	F5V3	TSF27	Speciation Factor, THC Class 27[a]
77	81	5	F5V3	TSF28	Speciation Factor, THC Class 28[a]
82	86	5	F5V3	TSF29	Speciation Factor, THC Class 29[a]
87	91	5	F5V3	TSF30	Speciation Factor, THC Class 30[a]
92	96	5	F5V3	TSF31	Speciation Factor, THC Class 31[a]
97	101	5	F5V3	TSF32	Speciation Factor, THC Class 32[a]
102	113	12	-	--	Unused
114	115	2	I	TYPE	Record Type (=22)

[a]For area source processing, these fields are left blank.
[b]Speciation factors are 5-digit numbers with an implied decimal point to the right of the second digit.
[c]Units are moles of the THC class per kilogram of total hydrocarbon.

"speciated" by both alkalinity and size fraction. Each of the four alkaline dust species in the inventory—calcium, magnesium, sodium, and potassium—is expressed in terms of 0 to 2.5 micron fraction, 2.5 to 10 micron fraction, and total species. In addition, TSP is speciated into three size ranges including 0 to 2.5, 2.5 to 6, and 6 to 10 micron components. As with NO_x factors, speciation factors for particulates are dimensionless weight fractions which are multiplied by TSP emissions to yield an estimate of the number of tons of each species class.

A complete listing of particulate species classes in the 1985 modeling inventory is shown in Table 4-3. Unlike other pollutants in the inventory, these classes cannot be uniquely defined using five-digit Storage and Retrieval of Aerometric Data (SAROAD) pollutant codes. In order to distinguish by both species and size fraction, a two-digit size class code was developed. The code is concatenated to the front of the species SAROAD code to create a unique seven-digit identifier. When input to FREDS, the two codes are interpreted as one for the purpose of TSP speciation.

Input File Development

Data for speciated particulate emissions were extremely limited during the early stages of NAPAP inventory development. For the 1980 inventory, TSP emissions were speciated into four alkaline dust categories; however, speciation factors were available for only 10 percent of all point source SCCs. Emission factors were developed by Meteorological and Environmental Planning Limited and the Ontario Research Foundation and incorporated into the inventory without change. Generic source descriptions used in development of the factors were matched to point source SCCs at the six-digit level. No attempt was made to speciate anthropogenic area source categories.

As in the case of hydrocarbons, Radian's *Air Emissions Species Manual* is the primary source of data for speciated particulate matter (PM) for the 1985 NAPAP inventory. The Radian study, conducted in support of NAPAP as well as PM_{10} source apportionment studies, consisted of an analysis of the profiles contained in the *Receptor Model Source Composition Library* (EPA, 1984) and the development of new profiles based on literature search efforts. The Radian data base consists of 131 "original" profiles, 11 composite profiles (which represent groupings of several profiles available for the same category), 16 industry-specific average (default) profiles, and an overall average or "zero" profile.

For each profile, the following data were compiled:

- *Composition data* for four size ranges: 0 to 2.5 um, 2.5 to 10 um, 0 to 10 um, and total particulate. These data are expressed as weight percent of the given size fraction occurring as a certain species.
- *Mass Fraction data* for the 0 to 2.5, 0 to 6, and 0 to 10 um size ranges. These represent the fraction of total particulate mass contained within the specific size range.

TABLE 4-3. PARTICULATE SPECIES CLASSES, 1985 NAPAP RESOLVED INVENTORY

Size class code	Species SAROAD code	Description
10[a]	12111[b]	Reactive calcium (Ca), 0-2.5 micron size range
30	12111	Reactive calcium, 2.5-10 micron size range
50	12111	Reactive calcium, total
10	12140	Reactive magnesium (Mg), 0-2.5 micron size range
30	12140	Reactive magnesium, 2.5-10 micron size range
50	12140	Reactive magnesium, total
10	12180	Reactive potassium (K), 0-2.5 micron size range
30	12180	Reactive potassium, 2.5-10 micron size range
50	12180	Reactive potassium, total
10	12184	Reactive sodium (Na), 0-2.5 micron size range
30	12184	Reactive sodium, 2.5-10 micron size range
50	12184	Reactive sodium, total
10	11101	Total particulates, 0-2.5 micron size range
20	11101	Total particulates, 2.5-6 micron size range
40	11101	Total particulates, 6-10 micron size range

[a]Size class codes are defined as follows:

Code	Size range (microns)
10	0 - 2.5
20	2.5 - 6.0
30	2.5 - 10.0
40	6.0 - 10.0
50	Total

[b]Species SAROAD codes are defined as follows:

SAROAD	Species
12111	Calcium (Ca)
12140	Magnesium (Mg)
12180	Potassium (K)
12184	Sodium (Na)
11101	Total particulates

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- *Reactivity data* for the alkaline particulate species (Na, K, Ca, and Mg). The "reactive fraction" is defined as that fraction of each element which is present as an oxide, carbonate, carbide, or hydroxide. These are species in which the cation is readily dissociated and available for reaction with acidic solutions.

In addition, as part of the profile development effort, Radian assigned all NEDS point and area source categories to particulate speciation profiles. The specific particulate classes required for RADM were selected by personnel from NCAR and EPA's Atmospheric Research and Exposure Assessment Laboratory (AREAL).

Speciation Factor File Generation and Quality Control

In order to convert the profile data into speciation factors suitable for NAPAP, the composition, mass fraction, and reactivity data must be combined so as to represent the reactive fraction of a given species within a given size fraction. For example, to calculate the speciation factor representing the reactive fraction of species X within size fraction Y for profile Z ($SF_{X,Y,Z}$), the following equation is used:

$$SF_{X,Y,Z} = \frac{1}{100} (WP_{X,Y,Z}) (MF_{Y,Z}) (RF_{X,Z}) \qquad (4.1)$$

where: $WP_{X,Y,Z}$ = weight percent of size fraction Y occupied by species X, profile Z;

$MF_{Y,Z}$ = mass fraction of total particulate occurring within size fraction Y, profile Z; and

$RF_{X,Z}$ = reactive fraction of species X, profile Z.

Two computer programs were developed to derive speciation factors from Radian data. The first program utilized the profile, fraction, and reactivity data to create speciation fractions using equation 4.1 above. The Radian profile data were reformatted and reduced to contain only the four species relevant to NAPAP (Na, Ca, K, and Mg), at the size ranges desired. These were multiplied by the fraction of total TSP occurring at each size range, and finally by the reactive fractions of the four species. The resulting "species-profile" file was used as input to a second program, which matched the speciation factors to source categories using SCC-profile index files, and wrote the resulting data set in FREDS-compatible EBCDIC format.

Quality control checks of the Radian particulate speciation data consisted of a series of manual and automated procedures designed primarily to detect problems which would prevent successful FREDS execution. Missing or invalid data elements, duplicate SCC-profile combinations and point source SCCs missing profile assignments were detected in early versions of the data. These were reported and subsequently corrected by Radian. Profile assignments for new NAPAP area source categories were made by Alliance. The PM default profile (0) was employed for the mobile source ammonia categories (66-68). Livestock waste management categories for turkeys and sheep (69 and 70) were assigned to profile 90003, (food and agriculture-industry average) consistent with Radian's assignments for the similar categories 70 through 75.

During early tests of speciation data, discrepancies between the mass of the speciated size fractions and the total species masses were discovered. Of the 159 particulate profiles, 20 were identified in which the sum of the 0 to 2.5 micron fraction and the 2.5 to 10 micron fraction exceeded the total species estimate. Examination of the profiles indicated that the problem was associated with the calculation of the total species fraction. In the absence of an algorithm with which to recalculate the fraction, the total species values were replaced with fractions representing the minimum allowable total species value. The 0 to 10 micron fraction was used for 15 of the 20 profiles; the remainder were calculated on a case-by-case basis. Although the procedure resulted in internal consistency for the profiles, it raises some concern as to the validity of other total mass fractions in the profiles.

Speciation Factor File Format

An example of Speciation Factor File format is shown in Table 4-4. The SFF can accommodate 20 speciation factors, 10 per line, and is formatted in a manner similar to the PSPLIT file. Each speciation factor is expressed as an eight-digit integer which is read into the FREDS Speciation Module with all digits to the right of the decimal. Seven digits are allowed for the species class codes in the file header to accommodate particulate size class/SAROAD code combinations.

HYDROCARBON PREPROCESSING

Background

Another important application of speciation data for the NAPAP inventory is the "preprocessing" of reported hydrocarbon emissions. While annual NEDS data report source-level emissions of Volatile Organic Compounds (VOC), the VOC estimates are often calculated on different bases, making quantitative comparisons of raw data prone to inaccuracy. For example, a source reporting "VOC" may or may not include methane in its estimate. Also, depending on the method used to estimate emissions, the presence of aldehydes may not be accounted for. Flame Ionization Detection (FID) is relatively insensitive to aldehydes; sources reporting hydrocarbons calculated using FID can, therefore, be assumed to lack a mass corresponding to the expected weight fraction of aldehydes.

To ensure internal consistency in handling organic compound emissions estimates, NAPAP processing software includes a Hydrocarbon Preprocessor which accepts a single reported annual hydrocarbon value and derives estimates of VOC and total hydrocarbons (THC) for each source in the inventory. The NAPAP Annual Emissions Inventory is the output of the Hydrocarbon Preprocessor. By definition, VOC and THC differ only by the expected mass of methane. Since methane is included in the speciation profiles used by FREDS, it is the THC value which is used in subsequent NAPAP hydrocarbon speciation steps.

TABLE 4-4. PARTICULATE SPECIATION FACTOR FILE FORMAT

Record position		Column width	Format	Variable name	Description
First	Last				
Header Record No. 1					
1	7	7	I	CLASS1	Pseudo-SAROAD code for TSP Class No. 1
6	14	7	I	CLASS2	Pseudo-SAROAD code for TSP Class No. 2
15	21	7	I	CLASS3	Pseudo-SAROAD code for TSP Class No. 3
22	28	7	I	CLASS4	Pseudo-SAROAD code for TSP Class No. 4
29	35	7	I	CLASS5	Pseudo-SAROAD code for TSP Class No. 5
36	42	7	I	CLASS6	Pseudo-SAROAD code for TSP Class No. 6
43	49	7	I	CLASS7	Pseudo-SAROAD code for TSP Class No. 7
50	56	7	I	CLASS8	Pseudo-SAROAD code for TSP Class No. 8
57	63	7	I	CLASS9	Pseudo-SAROAD code for TSP Class No. 9
64	70	7	I	CLASS10	Pseudo-SAROAD code for TSP Class No. 10
71	103	33	-	-	Unused
104	105	2	I	TYPE	Record Type (=11)
Header Record No. 2					
1	7	7	I	CLASS11	Pseudo-SAROAD code for TSP Class No. 11
8	14	7	I	CLASS12	Pseudo-SAROAD code for TSP Class No. 12
15	21	7	I	CLASS13	Pseudo-SAROAD code for TSP Class No. 13
22	28	7	I	CLASS14	Pseudo-SAROAD code for TSP Class No. 14
29	35	7	I	CLASS15	Pseudo-SAROAD code for TSP Class No. 15
36	42	7	I	CLASS16	Pseudo-SAROAD code for TSP Class No. 16
43	49	7	I	CLASS17	Pseudo-SAROAD code for TSP Class No. 17
50	56	7	I	CLASS18	Pseudo-SAROAD code for TSP Class No. 18
57	63	7	I	CLASS19	Pseudo-SAROAD code for TSP Class No. 19
64	70	7	I	CLASS20	Pseudo-SAROAD code for TSP Class No. 20
71	103	33	-	-	Unused
104	105	2	I	TYPE	Record Type (=12)
Speciation Record No. 1					
1	2	2	I	STATE	AEROS State Code
3	6	4	I	COUNTY	AEROS County Code
7	10	4	A	PLANT_ID	Plant Identification Code[a]
11	13	3	A	POINT_ID	Point Identification Code[a]
14	21	8	I	SCC	Area Source Category or Point Source SCC
22	29	8	F8V8[b]	TSF1	Speciation Factor for Class 1[a]
30	37	8	F8V8	TSF2	Speciation Factor for Class 2[a]
38	45	8	F8V8	TSF3	Speciation Factor for Class 3[a]
46	53	8	F8V8	TSF4	Speciation Factor for Class 4[a]
54	61	8	F8V8	TSF5	Speciation Factor for Class 5[a]
62	69	8	F8V8	TSF6	Speciation Factor for Class 6[a]
70	77	8	F8V8	TSF7	Speciation Factor for Class 7[a]

(continued)

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TABLE 4-4 (continued)

Record position		Column width	Format	Variable name	Description
First	Last				
78	85	8	F8V8	TSF8	Speciation Factor for Class 8[c]
86	94	8	F8V8	TSF9	Speciation Factor for Class 9[c]
95	102	8	F8V8	TSF10	Speciation Factor for Class 10[c]
103	103	1	-	-	Unused
104	105	2	I	TYPE	Record Type (=21)
Speciation Record No. 2					
1	2	2	I	STATE	AEROS State Code
3	6	4	I	COUNTY	AEROS County Code
7	10	4	A	PLANT_ID	Plant Identification Code[a]
11	13	3	A	POINT_ID	Point Identification Code[a]
14	21	8	I	SCC	Area Source Category or Point Source SCC
22	29	8	F8V8[b]	TSF11	Speciation Factor for Class 11[c]
30	37	8	F8V8	TSF12	Speciation Factor for Class 12[c]
38	45	8	F8V8	TSF13	Speciation Factor for Class 13[c]
46	53	8	F8V8	TSF14	Speciation Factor for Class 14[c]
54	61	8	F8V8	TSF15	Speciation Factor for Class 15[c]
62	103	41	-	-	Unused
104	105	2	I	TYPE	Record Type (=22)

[a]For area source runs, these fields are left blank.
[b]Speciation factors are 8-digit integers which are read into FREDS with all 8-digits to the right of the decimal point.
[c]Speciation factors are dimensionless weight fractions.

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Hydrocarbon preprocessing is performed at the source category (SCC) level, as is speciation, based on the mass fractions of formaldehyde and methane reported in the hydrocarbon species-profile file. Adjustment is controlled by a set of formaldehyde and methane flags which specify whether or not augmentation is to be performed for the SCC in question (1 = augment; 0 = do not augment). The flag settings depend on whether or not the source type is expected to have accounted for aldehydes and/or methane in its original emissions estimate.

An example of this methodology in practice is illustrated in Figure 4-1, on a hypothetical source which reports hydrocarbon emissions of 100 tons. The source category corresponds to a profile containing 10 percent methane and 5 percent formaldehyde by weight. An intermediate adjustment factor is calculated using the following equation:

$$\text{Adjustment factor} = \frac{\left(\begin{matrix}\text{formaldehyde} \\ \text{weight \%}\end{matrix} \times \begin{matrix}\text{formaldehyde} \\ \text{flag}\end{matrix}\right) + \left(\begin{matrix}\text{methane} \\ \text{weight \%}\end{matrix} \times \begin{matrix}\text{methane} \\ \text{flag}\end{matrix}\right)}{100} \qquad (4.2)$$

The adjustment factor represents the total mass fraction of species unaccounted for in the input hydrocarbon estimate. Actual THC can therefore be calculated as:

$$\text{Actual THC} = \frac{\text{Input hydrocarbon}}{1 - (\text{Adjustment factor})} \qquad (4.3)$$

VOC is then calculated by removing the mass fraction of methane from THC:

$$\text{Actual VOC} = \text{Actual THC} \times \frac{100 - (\text{methane weight \%})}{100} \qquad (4.4)$$

Figure 4-1 illustrates the four possible THC/VOC outcomes depending on the settings of the formaldehyde and methane flags.

File Development and Quality Assurance

Profile-specific weight percents for formaldehyde and methane were extracted from the Radian hydrocarbon speciation profiles discussed previously. Alliance conducted a review of these profiles and developed a set of augmentation recommendations which formed the basis for the aldehyde and methane flag values (Battye, 1987). Several general rules and assumptions were used in making the recommendations list, which are summarized below:

- Where a profile does not contain formaldehyde, augmentation for formaldehyde would have no effect. Therefore, a no-augment code generally was entered in these cases. The same rule was used for profiles that do not contain methane.

GIVEN:

Input hydrocarbon = 100 tons/year

Weight percent methane in profile = 10%

Weight percent formaldehyde in profile = 5%

GOVERNING EQUATIONS:

$$\text{Adjustment factor} = \frac{\left[\left(\begin{matrix}\text{formaldehyde}\\ \text{weight \%}\end{matrix}\right) \times \left(\begin{matrix}\text{formaldehyde}\\ \text{flag}\end{matrix}\right)\right] + \left[\left(\begin{matrix}\text{methane}\\ \text{weight \%}\end{matrix}\right) \times \left(\begin{matrix}\text{methene}\\ \text{flag}\end{matrix}\right)\right]}{100}$$

$$= \frac{[5 \times (\text{formaldehyde flag})] + [10 \times (\text{methane flag})]}{100}$$

$$\text{Actual THC} = \frac{\text{Input hydrocarbon}}{1 - (\text{adjustment factor})} = \frac{100 \text{ tons/year}}{1 - (\text{adjustment factor})}$$

$$\text{Actual VOC} = \text{Actual THC} \times \frac{100 - (\text{methane weight \%})}{100} = \text{Actual THC} \times (0.9)$$

RESULTS:

Methane flag	Aldehyde flag	Adjustment factor	Calculated emissions, tons/year	
			THC	VOC
0	0	0.00	100.0	90.0
0	1	0.05	105.3	94.7
1	0	0.10	111.1	100.0
1	1	0.15	117.6	105.9

Figure 4-1. Example of VOC and THC calculation, FREDS Hydrocarbon Preprocessor.

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- For all point source combustion categories, VOC emissions were assumed to be based on flame ionization detector measurements of total hydrocarbons, in which methane would not have been broken out from other hydrocarbons and formaldehyde would not have been detected. A similar assumption was made for VOC emissions from metallurgical processes. Thus, for these categories, it was recommended that emissions be augmented for formaldehyde, but not for methane.

- For petrochemical vents containing formaldehyde, it was assumed that a detection technique was used that is suited to formaldehyde. It was also assumed that the formaldehyde content of petrochemical process streams was known, and hence that fugitive VOC emissions estimates include formaldehyde where appropriate. It was assumed that VOC emissions estimates for petrochemical processes did not include methane. Thus, it was recommended that petrochemical process vent emissions and fugitive emissions be augmented for methane, but not for formaldehyde.

- For area source categories in general, emissions estimates were assumed to be derived from detailed compound-specific measurements. Thus, it was assumed that VOC emissions estimates for these categories include formaldehyde and do not include methane. Augmentation was therefore recommended for methane and not for formaldehyde.

Following EPA review, the flags were merged to the profile-specific weight percents of formaldehyde and methane to form the augmentation file used by the Hydrocarbon Preprocessor. The file is illustrated in Table 4-5.

Preliminary testing uncovered a problem with the flag settings for the profile representing residential natural gas combustion. AP-42 listed both a methane and a non-methane hydrocarbon emission factor for this source type (5.3 and 2.7 lb/million ft^3, respectively), and a methane augmentation was recommended. The Radian data, however, indicated that the profile was 100 percent methane. The resulting adjustment factor of 1.00 would cause a division-by-zero condition in equation 4.3, and could not be processed by NAPAP software. The methane flag for this profile was therefore changed to zero prior to final inventory processing.

TABLE 4-5. HYDROCARBON AUGMENTATION FLAG FILE

Profile number	Methane wt. pct.	Formaldehyde wt. pct.	Formaldehyde flag	Methane flag
0	7.36	1.55	0	0
1	11.00	42.00	1	0
2	0.00	48.70	1	0
3	56.00	8.00	1	0
4	7.60	7.60	1	0
5	82.80	0.00	1	0
7	70.00	30.00	1	0
8	11.60	0.00	1	0
9	11.60	0.00	1	0
11	45.30	0.00	1	0
12	15.80	0.00	1	0
13	73.30	0.00	1	0
14	0.00	0.00	1	0
16	11.10	0.00	1	0
23	0.00	0.00	1	0
24	21.30	0.00	1	0
25	56.00	8.00	1	0
26	15.70	0.00	1	0
29	36.00	51.00	1	0
31	2.90	0.00	1	0
35	0.00	0.00	1	0
39	13.30	0.00	1	0
47	0.00	0.00	1	0
51	20.00	20.00	1	0
66	0.00	0.00	0	0
68	0.00	0.00	0	0
72	0.00	0.00	0	0
76	0.00	0.00	0	0
78	0.00	0.00	0	0
79	0.00	1.70	1	0
85	0.00	0.00	0	0
87	0.00	0.00	0	0
88	0.00	0.00	0	0
89	0.00	0.00	0	0
90	0.00	0.00	0	0
100	0.00	0.00	0	0
121	0.00	0.00	0	0
122	80.40	0.00	1	0
127	0.00	0.00	1	0
166	63.00	0.00	0	0
182	0.00	0.00	0	0
183	0.00	0.00	0	0
195	100.00	0.00	1	0
197	0.00	0.60	0	0
202	98.70	0.00	1	0
203	70.00	0.00	0	1
217	40.90	0.00	1	0
219	0.00	0.00	0	0
220	0.00	0.00	0	0
221	0.00	0.00	0	0
222	0.00	0.00	0	0

(continued)

TABLE 4-5 (continued)

Profile number	Methane wt. pct.	Formaldehyde wt. pct.	Formaldehyde flag	Methane flag
223	0.00	0.00	0	0
225	0.00	0.00	0	0
226	0.00	0.00	0	0
227	0.00	0.00	0	0
228	0.00	0.00	0	0
229	0.00	0.00	0	0
230	0.00	0.00	0	0
271	0.00	0.00	0	0
272	0.00	0.00	0	0
273	0.00	0.00	0	0
274	0.00	0.00	0	0
275	0.00	0.00	0	0
277	0.00	0.00	0	0
282	0.00	0.00	0	0
288	0.00	0.00	0	0
289	0.00	0.00	0	0
290	0.00	0.00	0	0
291	0.00	0.00	0	0
292	0.00	0.00	0	0
296	6.20	0.00	0	0
297	8.80	0.00	0	0
299	0.00	0.00	0	0
301	0.00	0.00	0	0
304	0.00	0.00	0	0
305	2.60	0.00	0	0
307	9.82	0.00	1	1
316	28.60	0.00	1	0
321	3.30	0.00	1	0
332	17.10	21.80	0	0
333	37.66	0.00	0	0
1001	76.69	0.81	1	0
1002	22.40	0.00	1	0
1003	0.00	0.00	0	0
1004	0.00	0.00	0	0
1005	0.00	0.00	0	0
1006	0.00	0.00	0	0
1007	0.00	0.00	1	0
1008	0.00	0.00	0	0
1009	0.00	0.00	0	0
1010	46.31	0.00	0	0
1011	37.60	0.00	0	0
1012	61.30	0.00	0	0
1013	0.00	0.00	0	0
1014	0.00	0.00	0	0
1015	0.00	0.00	0	0
1016	0.00	0.00	0	0
1017	0.00	0.00	0	0
1018	0.00	0.00	0	0
1019	0.00	0.00	0	0
1020	0.00	0.00	0	0
1021	0.00	0.00	0	0

(continued)

TABLE 4-5 (continued)

Profile number	Methane wt. pct.	Formaldehyde wt. pct.	Formaldehyde flag	Methane flag
1022	0.00	0.00	0	0
1023	0.00	0.00	0	0
1024	0.00	0.00	0	0
1025	17.23	0.00	0	0
1026	0.00	0.00	0	0
1027	0.00	0.00	0	0
1028	0.00	0.00	0	0
1029	0.00	0.00	0	0
1030	4.28	0.00	0	0
1031	0.00	0.00	0	0
1032	0.00	0.00	0	0
1033	0.00	0.00	0	0
1034	0.00	0.00	0	0
1035	0.00	0.00	0	0
1036	0.00	0.00	1	0
1037	18.35	0.00	0	1
1038	3.73	0.00	0	1
1039	12.94	0.00	0	1
1040	0.00	0.00	0	1
1041	0.00	0.00	0	1
1042	0.00	0.00	0	1
1043	0.00	0.00	0	1
1044	0.00	0.00	0	1
1045	0.00	0.00	0	1
1046	4.88	0.00	0	1
1047	0.00	0.00	0	1
1048	0.00	0.00	0	1
1049	16.07	0.00	0	1
1050	0.00	0.00	0	1
1051	0.00	0.00	0	1
1052	0.00	0.00	0	1
1053	0.00	0.00	0	1
1054	0.00	0.00	0	1
1055	0.00	0.00	0	1
1056	0.00	0.00	0	1
1057	52.30	0.00	0	1
1058	24.38	0.00	0	1
1059	1.79	0.00	0	1
1060	0.00	0.00	0	1
1061	0.00	0.00	0	1
1062	0.00	0.00	0	1
1064	12.46	0.00	0	1
1065	0.51	0.00	0	1
1066	21.73	0.00	0	1
1067	34.72	0.00	0	1
1068	0.00	0.00	0	1
1069	0.00	0.00	0	1
1070	86.71	0.00	0	0
1071	0.00	0.00	0	0
1072	0.00	0.00	0	1
1073	0.00	0.00	0	1

(continued)

TABLE 4-5 (continued)

Profile number	Methane wt. pct.	Formaldehyde wt. pct.	Formaldehyde flag	Methane flag
1074	0.00	0.00	0	1
1075	0.00	0.00	0	1
1076	0.00	0.00	0	1
1077	0.00	0.00	0	1
1078	0.00	0.00	0	1
1079	0.00	0.00	0	1
1080	0.00	0.00	0	1
1081	0.00	0.00	0	1
1082	0.00	0.00	0	1
1083	0.00	0.00	0	1
1084	38.39	0.00	1	0
1085	20.00	0.00	1	0
1086	0.00	0.00	0	0
1087	0.00	0.00	0	1
1088	0.00	0.00	0	0
1089	0.00	0.70	1	0
1090	0.00	0.00	0	1
1091	0.00	0.00	0	1
1092	0.00	0.00	0	1
1093	0.00	0.00	0	1
1094	0.00	0.00	0	1
1095	0.00	0.00	0	1
1096	0.00	0.00	0	1
1097	9.38	15.49	1	0
1098	9.57	15.01	1	0
1099	10.95	14.14	1	0
1100	0.00	0.00	0	0
1101	10.07	0.74	1	1
1103	0.00	0.00	0	0
1104	0.00	0.00	0	0
1105	0.00	0.00	0	0
1106	0.00	0.00	0	0
1107	0.00	0.00	0	0
1108	0.00	0.00	0	0
1109	0.00	0.00	0	0
1110	0.00	0.00	0	0
1111	0.00	0.00	0	0
1112	0.00	0.00	0	0
1114	0.00	0.00	0	0
1115	0.00	0.00	0	0
1116	0.00	0.00	0	0
1118	0.00	0.00	0	0
1119	0.00	0.00	0	0
1120	0.00	0.00	0	0
1121	0.00	0.00	0	0
1122	0.00	0.00	0	0
1123	0.00	0.00	0	0
1124	0.00	0.00	0	0
1125	0.00	0.00	0	0
1126	0.00	0.00	0	0
1127	0.00	0.00	0	0

(continued)

TABLE 4-5 (continued)

Profile number	Methane wt. pct.	Formaldehyde wt. pct.	Formaldehyde flag	Methane flag
1128	0.00	0.00	0	0
1129	0.00	0.00	0	0
1130	0.00	0.00	0	0
1131	0.00	0.00	0	0
1132	0.00	0.00	0	0
1134	0.00	0.00	0	0
1135	0.00	0.00	0	0
1136	0.00	0.00	0	0
1137	0.00	0.00	0	0
1138	0.00	0.00	0	0
1139	0.00	0.00	0	0
1140	0.00	100.00	0	0
1141	0.00	0.00	0	0
1142	0.00	0.00	0	0
1144	0.00	0.00	0	0
1145	0.00	0.00	0	0
1146	0.00	0.00	0	0
1147	0.00	0.00	0	0
1148	0.00	0.00	0	0
1149	0.00	0.00	0	0
1150	0.00	0.00	0	0
1151	0.00	0.00	0	0
1152	0.00	0.00	0	0
1153	0.00	0.00	0	0
1154	0.00	0.00	0	0
1155	0.00	0.00	0	0
1158	0.00	0.00	0	0
1159	0.00	0.00	0	0
1160	0.00	0.00	0	0
1162	0.00	0.00	0	0
1163	0.00	0.00	0	0
1164	0.00	0.00	0	0
1165	0.00	0.00	0	0
1166	0.00	0.00	0	0
1167	0.00	0.66	1	1
1168	0.00	0.00	0	0
1171	0.00	0.00	0	0
1172	0.00	0.00	0	0
1173	0.00	0.00	0	0
1174	0.00	0.00	0	0
1175	0.00	0.00	0	0
1176	0.00	0.00	0	0
1178	0.00	0.00	1	0
1185	0.00	0.00	1	0
1186	2.45	0.00	1	1
1187	0.00	0.00	0	0
1188	0.00	0.00	0	0
1189	0.00	0.00	1	0
1190	0.00	0.00	0	0
1191	0.00	0.00	0	0
1192	0.00	0.00	0	0

(continued)

TABLE 4-5 (continued)

Profile number	Methane wt. pct.	Formaldehyde wt. pct.	Formaldehyde flag	Methane flag
1193	0.00	0.00	0	0
1194	0.00	0.00	0	0
1195	0.00	0.00	0	0
1196	0.00	0.00	0	0
1197	0.00	0.00	0	0
1198	0.00	0.00	0	0
1199	0.00	0.00	0	0
1200	0.00	0.00	0	0
1201	4.40	12.20	0	1
1202	0.00	0.00	0	0
1203	10.97	1.42	1	1
1204	0.04	0.00	1	1
9001	25.35	15.19	1	0
9002	42.45	7.70	1	0
9003	9.02	1.82	0	1
9004	5.07	0.03	0	1
9005	0.00	0.00	0	1
9006	0.00	0.00	0	1
9007	43.35	0.00	0	1
9008	0.00	0.00	1	0
9009	29.10	0.00	1	0
9010	0.00	0.35	1	0
9011	18.60	1.60	1	0
9012	13.01	8.88	1	0
9013	0.00	0.00	1	0
9014	0.00	0.00	0	1
9015	53.81	0.00	1	0
9016	0.00	0.00	0	0
9017	0.00	0.00	0	0
9021	0.00	0.00	0	0
9022	59.71	0.00	1	0
9023	0.00	0.00	0	0
9024	2.01	0.00	0	0
9025	3.02	0.00	0	0
9026	10.01	2.73	0	0
9027	1.30	0.00	0	0
9028	0.00	1.47	0	0
9029	0.00	0.00	0	0
9030	0.00	0.00	0	0
9031	0.00	0.00	0	0
9032	0.00	0.00	0	0
9033	0.00	0.00	0	0
9034	0.00	0.00	0	0
9035	0.00	0.00	0	0
9036	0.00	0.00	0	0
9037	0.00	0.00	0	0
9038	0.00	0.00	0	0
9039	0.00	0.00	0	0
9040	0.00	0.00	0	0
9041	0.00	25.00	0	0

(continued)

TABLE 4-5 (continued)

Profile number	Methane wt. pct.	Formaldehyde wt. pct.	Formaldehyde flag	Methane flag
9042	0.00	0.00	0	0
9043	0.00	0.00	0	0
9044	0.00	0.00	0	0
9046	0.00	0.00	0	0
9047	0.00	0.00	0	0

SECTION 5

REFERENCES

GENERAL REFERENCES

Demmy, J.L., W.M. Tax, and T.E. Warn. Area Source Documentation for the 1985 National Acid Precipitation Assessment Program Inventory. EPA-600/8-88-106 (NTIS PB89-151427), U.S. Environmental Protection Agency, Research Triangle Park, NC. December 1988.

Lebowitz, L.G., and A.S. Ackerman. Flexible Regional Emissions Data System (FREDS) Documentation for the 1980 NAPAP Emissions Inventory. EPA-600/7-87-025a (NTIS PB88-129499). U.S. Environmental Protection Agency, Research Triangle Park, NC. November 1987.

Middleton, P. Analysis of Emissions Databases for Regional Models. Atmos. Environ. 21:1497-1509. 1987.

Modica (Lebowitz), L.G., D.R. Dulleba, R.A. Walters, and J.E. Langstaff. Flexible Regional Emissions Data System (FREDS) Documentation for the 1985 NAPAP Emissions Inventory. EPA-600/9-89-047 (NTIS PB89-198816). U.S. Environmental Protection Agency, Research Triangle Park, NC. May 1989.

Sellars, F.M., T.E. Fitzgerald, Jr., J.M. Lennon, L.J. Maiocco, N.M. Monzione, and D.R. Neal, Jr. National Acid Precipitation Assessment Program Emission Inventory Allocation Factors, EPA-600/7-85-035 (NTIS PB86-104247), U.S. Environmental Protection Agency, Research Triangle Park, NC. September 1985.

U.S. Environmental Protection Agency. Compilation of Air Pollutant Emission Factors, Volume I: Stationary Point and Area Sources. AP-42. Fourth Edition. (GPO No. 055-000-00251-7), U.S. Environmental Protection Agency, Research Triangle Park, NC. September 1985.

Wagner, J. K., R. A. Walters, L. J. Maiocco, and D. R. Neal. Development of the 1980 NAPAP Emissions Inventory. EPA-600/7-86-057a (NTIS PB88-132121), U.S. Environmental Protection Agency, Research Triangle Park, NC. December 1986.

Zimmerman, D., W. Tax, M. Smith, J. Demmy, and R. Battye. Anthropogenic Emissions Data for the 1985 NAPAP Inventory. EPA-600/7-88-022 (NTIS PB89-151419), U.S. Environmental Protection Agency, Air and Energy Engineering Research Laboratory, Research Triangle Park, NC. November 1988.

TEMPORAL FACTOR REFERENCES

Electric Power Research Institute. The EPRI Regional Systems. EPRI P-1950-SR. Palo Alto, CA. 1981.

Engineering-Science. Emissions Inventories for Urban Airshed Model Application in the Philadelphia AQCR. Prepared for the U.S. Environmental Protection Agency. EPA-450/4-82-005 (NTIS PB83-187823). Research Triangle Park, NC. April 1982.

Klemm, H. A. and R. J. Brennan. Emissions Inventory for the SURE Region. Alliance Technologies Corporation for the Electric Power Research Institute, EA-1913. Palo Alto, CA. 1981.

Sellars, F., et al. Northeast Corridor Regional Modeling Project Annual Emission Inventory Compilation and Formatting. GCA Technology Division for the U.S. Environmental Protection Agency. EPA-450/4-82-013a-r. Research Triangle Park, NC. 1982.

U.S. Department of Commerce. Local Climatological Data Published Stations (1980 data), National Climatic Data Center, National Oceanic and Atmospheric Administration. Asheville, NC. 1980.

U.S. Department of Commerce. State, Regional, and National Monthly and Annual Temperatures Weighted by Area. Historical Climatology Series 4-1. National Oceanic and Atmospheric Administration. Asheville, NC. 1983a.

U.S. Department of Commerce. State, Regional, and National Monthly and Seasonal Heating Degree Days Weighted by Population (1980 Census). Historical Climatology Series 5-1. National Oceanic and Atmospheric Administration. Asheville, NC. 1983b.

U.S. Department of Energy. Energy Data Reports, Washington, D.C., 1979.

U.S. Department of Energy. Petroleum Marketing Monthly. Energy Information Service. Washington, D.C. 1984.

U.S. Environmental Protection Agency. 1979a. Documentation of the Regional Air Pollution Study (RAPS) and Related Investigations in the St. Louis Air Quality Control Region. EPA-600/4-79-076 (NTIS PB80-138241). Research Triangle Park, NC. 1979.

U.S. Environmental Protection Agency, 1979b. Procedures for the Preparation of Emission Inventories for Volatile Organic Compounds; Volume II--Emission Inventory Requirements for Photochemical Air Quality Simulation Models. EPA-450/4-79-018 (NTIS PB80-202229), Research Triangle Park, NC. 1979.

U.S. Environmental Protection Agency. Emission Inventories for Urban Airshed Model Application in Tulsa, Oklahoma. EPA-450/4-80-021 (NTIS PB81-156986). Research Triangle Park, NC. 1980.

U.S. Environmental Protection Agency. Technical Tables to the National Air Pollutant Emissions Estimates, 1940-1984. EPA-450/4-85-014 (NTIS PB86-121100). Office of Air Quality Planning and Standards, Research Triangle Park, NC. January 1986.

U.S. Department of Labor. Supplement of Employment and Earnings: Revised Establishment Data, Bureau of Labor Statistics, Washington, D.C. 1981.

U.S. Department of Transportation, Federal Highway Administration. Highway Statistics. 1980 Annual.

SPATIAL FACTOR REFERENCES

Beaulieu, T.A., and L.G. Modica (Lebowitz). Documentation of Spatial Allocation Factor Procedures for the 1980 NAPAP Emissions Inventory. EPA-600/7-88-024a (NTIS PB89-159479), U.S. Environmental Protection Agency, Research Triangle Park, NC. December 1988.

U.S. Bureau of the Census, Census of Population and Housing, 1980: Master Area Reference File (MARF)2 [machine-readable data file]/prepared by the Bureau of Census. Washington: The Bureau [producer and distributer]. 1983.

U.S. Bureau of the Census, Census of Population and Housing, 1980: Summary Tape File 3 Technical Documentation. Prepared by the Data User Services Division, Bureau of the Census. Washington: The Bureau. pp. 437. 1982.

SPECIATION FACTOR REFERENCES

Compilation of Air Pollutant Emission Factors, Volume I: Stationary Point and Area Sources. AP-42. Fourth Edition (GPO No. 055-000-00251-7), U.S. Environmental Protection Agency, Research Triangle Park, NC, September 1985.

Core, J.E., J.J. Shah, J.A. Cooper. Receptor Model Source Composition Library. Nero & Associates and NEA, Inc. for the U.S. Environmental Protection Agency, EPA 450/4-85-002 (NTIS PB85-228823). November 1984.

Shareef, G., W. Butler, L. Bravo, and M. Stockton. Air Emissions Species Manual Volume I - Volatile Organic Compound (VOC) Species Profiles. EPA-450/2-88-003a (NTIS PB88-225792), U.S. Environmental Protection Agency, Research Triangle Park, NC. April 1988.

Shareef, G., and L. Bravo. Air Emissions Species Manual Volume II - Particulate Matter (PM) Species Profiles. EPA-450/2-88-003b (NTIS PB88-225800). U.S. Environmental Protection Agency, Research Triangle Park, NC. April 1988.

Volatile Organic Compound (VOC) Species Data Manual - Second Edition. Report No. EPA-450/4-80-015 (NTIS PB81-119455), U.S. Environmental Protection Agency, Research Triangle Park, NC. July 1980.

APPENDIX A

ADJUSTMENTS TO SPATIAL FRACTIONS FOR 1985 NAPAP PROCESSING

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ADJUSTMENTS TO SPATIAL FRACTIONS FOR 1985 NAPAP PROCESSING

Based on quality control procedures, adjustments were made to the existing spatial fractions for use with the 1985 NAPAP inventory. Corrections applied to the spatial fraction file are discussed below.

MISSING COUNTIES

Census-based spatial allocation factors (SAFs), i.e., population and housing, for the six Virginia counties/independent cities (Nansemond is the only Virginia county equivalent which is not an independent city) and Barbour, WV were available from another project. These data were input to the spatial fraction file. Since population is used as the default surrogate for NAPAP processing, these data are sufficient to spatially allocate emissions from these counties and independent cities.

To generate spatial fractions for Cibola, New Mexico, fractions developed for Valencia county were adjusted to account for the new county boundary, since Cibola was part of Valencia in 1980. Using the total population, housing, and land area fractions for Valencia along with the corresponding spatial fractions, population, housing and land area totals by grid cell were determined. These surrogates were then reaggregated separately for Cibola and Valencia and new population, housing, and land area fractions were calculated for each county. The remainder of the spatial category fields were assigned values of zero.

The remaining two missing counties, Sabine and Menominee, required a more detailed effort to generate gridded spatial fractions. Since population fractions could not be estimated for Sabine and Menominee, land area fractions were calculated. Since population is the default surrogate for NAPAP, these spatial fractions were inserted into the population field of the spatial fraction file.

MISSING GRID CELLS

For spatial allocation of emissions to missing grid cells for 1985 NAPAP processing, gridded population and housing fractions were calculated. Population and housing fractions for Queen Annes, MD for the two missing grid cells were available from a previous project. These values summed exactly to the fraction missing. Alexander, IL had only one missing grid cell, therefore, the calculated missing fractions for population and housing were assigned to that grid cell.

In Monroe, FL, and Dare, NC, the calculated missing fractions required allocation over several grid cells. To determine, as accurately as possible, the population distribution over these grid cells, population totals for each grid cell were determined using available town populations in each county. The grid cell coordinates for each town were calculated from the latitude and longitude of each town and the fractional population of each missing grid cell was estimated.

The population fraction for each town/grid was calculated by multiplying the fractional population of each missing grid cell by the missing population fraction from the SAFP processing messages. Spatial fractions for the same grid cell were combined. For Monroe County, SAFs for grid cells outside the NAPAP grid were kept such that the county's emissions could be correctly allocated.

COUNTY CODE ASSIGNMENTS

Incorrect county code assignments in the Saginaw County spatial data resulted from the presence of two different county codes in the land use file: 4600 and 4780. In the FIPAEROS file (and hence, census spatial file), Saginaw is coded as county 4600. In the emissions file, however, Saginaw is coded as 4780. This was further verified using the AEROS Manual (U.S. EPA, 1986). To assure correct spatial allocation of Saginaw's emissions, records with a county code of 4780 were deleted and records with a county code of 4600 were recoded to 4780 since these contained the complete census and land use fractions for each grid cell in Saginaw. The resultant spatial fractions are compatible with the area source emissions file.

For the Oregon and South Dakota counties, population and housing fractions were dropped in SPACEMERGE due to incorrect county code assignments. In Oregon, the county code assignments for Lincoln and Linn were switched in the land use county-to-grid file such that grid cells belonging to Lincoln were assigned to Linn, and vice-versa. As a result, when the census spatial surrogates were matched to the land use file, the census data was dropped due to no matching grids. Since the census data was dropped, population and housing values could not be retrieved. Thus, when the county codes for Lincoln and Linn were interchanged to the correct codes, the census fields still contained zero values. Since population is used as a default surrogate for NAPAP, values of land area were inserted into the population field to serve as the default surrogate for these counties.

In the census data, Jackson and Washabaugh counties were treated as a single entity (coded as Jackson - 0880). In the land use and emissions files, however, these were treated as separate counties. Thus, when the land use and census surrogates were merged, the census grids corresponding to Washabaugh county were dropped. The census-based spatial surrogates for Jackson are relative to the total of both counties and are, therefore, incorrect. Since the information necessary to correct the factors was not available, population values in both counties were substituted by land area fractions; housing fractions were set to zero.

LOCATION DATA

Spatial factor problems due to incorrect location data in the census files were noted for two Virginia counties (Pulaski and Rappahannock) and Adams, WI. In Pulaski, an independent city (Manassas) was assigned the NEDS code for this county. Manassas, however, is located in a different county (Prince William), in a different part of the State. The effect of this on Pulaski is census spatial surrogates off by more than 20 percent. To correct this, the grids located in Pulaski will be normalized by SAFP, thereby removing Manassas from the Pulaski county total.

In Rappahannock, latitude and longitude data for a subcounty census record corresponds to a grid cell outside the county border. As a result, the population and housing values for this grid cell were dropped in SPACEMERGE and the resultant county total for these surrogates is off by approximately 20 percent. To correct this, Rappahannock grid cells with zero population and housing values were identified. Two such cases existed, however, only one of the grids contained a town. The missing population and housing fractions were assigned to that grid cell.

Latitude and longitude data contained in the census data county and subcounty records for Adams, WI do not correspond to grid cells in the county. As a result, when the land use and census surrogates were merged, the census data was dropped by SPACEMERGE. The missing census population and housing fractions cannot be retrieved, however, land use fractions were available and, therefore, land area fractions were substituted in the population field to act as the default surrogate.

MASSACHUSETTS

A problem with the assignment of Massachusetts grid cells to Air Pollution Control Districts (APCDs) was discovered for categories spatially allocated by land use surrogates. Examination of the data files and software at various points in the spatial development process revealed a problem with the resolution of the spatial factors relative to the resolution of the reported emissions for Massachusetts. The land use spatial factors were developed relative to NAPAP county/grid cell information; i.e., the fraction of each county's land use contained within each grid cell. Massachusetts' emissions data are typically reported by APCD. When converting from county to APCDs, the land use fractions were not correctly transformed from county/grid cell resolution to APCD/grid cell resolution.

To correct this problem, a new set of land area spatial factors was developed for Massachusetts. The fractions were combined to form all unique APCD, column, and row combinations necessary for input to the Spatial Allocation Factor Preprocessor (SAFP). To incorporate the newly developed Massachusetts land area fractions

into the Spatial Fraction File, the old Massachusetts land area fractions were set to zero, and the new fractions merged into the file. Because information was not readily available to accurately correct the remaining land use surrogates, all other land use surrogates to be utilized by FREDS were set equal to the new land area fractions.

ALGORITHMS

Problems discovered with algorithms in CREATE5A, SPACEMERGE, and SAFP are summarized in Table 3-3. Minor problems with algorithms include: calculating column and row numbers for border grids for a subset of the NAPAP grid (CREATE5A), calculating column and row from grid number (SPACEMERGE), and normalization of county-level factors not summing to 100 percent (SAFP). The necessary corrections and changes to the spatial processing software were applied for future spatial factor processing.

NEW AREA SOURCE CATEGORIES

For 1985 NAPAP processing, ten new area source categories were created. Spatial allocation of emissions from these categories was accomplished by assigning surrogates to each category based on the existing 14 NAPAP surrogates. For each category, a surrogate was assigned based on activity levels used for characterization of emissions (Demmy, et al., 1987) and engineering judgment. The SCCs and surrogates corresponding to each category were included in the surrogate selection file prior to execution of SAFP. The assigned surrogates for each SCC are given in Table 3-2.

REFERENCES

U.S. Environmental Protection Agency. AEROS Manual Series, Volume V: AEROS Manual of Codes (3rd ed.). EPA-450/2-76-005b. Research Triangle Park, NC. April 1986.

Demmy, J.L., W.M. Tax, and T.E. Warn. Area Source Documentation for the 1985 National Acid Precipitation Assessment Program Inventory. EPA-600/8-88-106 (NTIS PB89-151427). U.S. Environmental Protection Agency, Research Triangle Park, NC. December 1988.

APPENDIX B

DEVELOPMENT OF ALLOCATION FACTORS FOR CANADIAN ANTHROPOGENIC SOURCES

APPENDIX B

DEVELOPMENT OF ALLOCATION FACTORS FOR CANADIAN ANTHROPOGENIC SOURCES

INTRODUCTION

Environment Canada, provincial air pollution control agencies, and the U.S. Environmental Protection Agency worked cooperatively to develop an annual inventory of Canadian emissions which would be consistent and compatible with the U.S. inventory. The Canadian data include emissions for 729 plants and 154 area source categories for 10 Provinces. The data are derived from a national inventory compiled by Environment Canada from data collected by provincial air pollution control agencies. Because the NAPAP geographic domain extends only to 60° north latitude, emissions data from the Yukon and Northwest Territories were reported to the U.S. EPA but were not processed for use by NAPAP. In addition, to ensure consistency between the two national inventories, only the 129 area source categories having analogs in the U.S. data were retained in the NAPAP Canadian file.

In order to allocate Canadian emissions data in a manner consistent with the allocation of U.S. anthropogenic emissions, Environment Canada also supplied data on spatial and temporal emissions patterns. Point source annual emissions were assigned to U.S. SCCS to allow speciation using the methodologies developed for the U.S. NAPAP inventories. The remainder of this section describes the allocation of Canadian point and area source inventories with particular emphasis on areas in which U.S. and Canadian methodologies differ.

TEMPORAL ALLOCATION FACTORS

Canadian emissions data files were accompanied by separate files containing temporal fractions for point and area sources. Temporal files contained throughput percentages for months of the year, days of the week, and hours of the day, respectively. Identifiers in these files permitted the merging of individual temporal scenarios into profiles compatible with sources in the emissions data files.

Separate temporal factor files were developed for point and area sources. For point sources, most factors were relative to the plant level. If data were collected at the point level, the profile for the point having the greatest emissions was used to allocate emissions for the entire plant. Area source factors were developed at the source category level. For both point and area sources, uniform default profiles were substituted when

temporal data were not available (DesLauriers, M. personal communication with D. Fratt, Alliance, March, 1989).

For FREDS processing, the temporal factors were reformatted to a form similar to the factors used for the U.S. NAPAP inventories. This required converting monthly throughputs to seasonal factors and weekday (Monday through Friday) fractions to an average value representing a typical weekday. File formats (Tables B-1 and B-2) are similar to those for U.S. point and area sources (Tables 2-2, 2-3), except that a record identifier (YWD) is required to link temporal profile records with emissions data. Twelve temporal scenarios are represented in each profile; one each for a typical weekday, Saturday and Sunday in each season (See Table 2-4). All files are stored as SAS data sets.

SPATIAL ALLOCATION FACTORS

Spatial allocation surrogates provided by Environment Canada included population, oil homes, gas homes, total homes, industrial labor force, commercial labor force, agricultural labor force and mining labor force. These data files were supplied to Environment Canada by Statistics Canada, and represent the 1981 base year. Census data for 1986 was also provided by Statistics Canada, but only data for population and total homes were available. To calculate spatial fractions, the census data were summed for each Province to obtain provincial totals, and the value for each grid cell was divided by the provincial total. Once the fractions were calculated, each of the Canadian area source categories was matched to the most appropriate surrogate category based on an analysis of the 1980 allocation factors, creating the Canadian surrogate selection file. A listing of Canadian area source categories and the assigned spatial surrogates are presented in Table B-3.

For final processing, the Spatial Allocation Factor Preprocessor (SAFP), used for processing the U.S. area source data, was modified to process the Canadian area source data. SAFP matches a spatial fraction for each grid cell to each area source category based on the surrogate selection file for later processing into a gridded, resolved inventory by FREDS. As with the U.S. data, the population surrogate was used as the default category for Canadian area source categories which either lacked a specific allocation surrogate or for which the assigned surrogate equaled zero when summed at the Province level. The file format for the EBCDIC Spatial Allocation Factor File input to FREDS is presented in Table B-4.

SPECIATION FACTORS

Canadian point and area source data were speciated using the data developed by Radian Corporation (Shareef, et. al., 1988). The Canadian point source data submittals included several SCC process classifications which had not been used in the U.S. data. The data processing for input into acid deposition models requires that a TSP and THC speciation profile be associated with every SCC included in the file. Therefore, Environment Canada requested that EPA make appropriate speciation profile assignments for those SCCs. In some cases,

TABLE B-1. FORMAT OF SAS DATA SET CONTAINING TEMPORAL ALLOCATION FACTORS FOR 1985 CANADIAN AREA SOURCE EMISSIONS DATA

Variable name	SAS variable length (bytes)	Description
NUM_DAY	8	Temporal Scenario Code
TWD	8	Profile Identifier
SEA	8	Seasonal Temporal Allocation Factor
DAY	8	Daily Temporal Allocation Factor
HOUR1-HOUR24	8	Hourly Temporal Allocation Factors

TABLE B-2. FORMAT OF SAS DATA SET CONTAINING TEMPORAL ALLOCATION FACTORS FOR 1985 CANADIAN POINT SOURCE EMISSIONS DATA

Variable name	SAS variable length (bytes)	Description
NUM_DAY	8	Temporal Scenario Code
YWD	8	Profile Identifier
SEA1-SEA12	8	Seasonal Temporal Allocation Factors
DAY1-DAY12	8	Daily Temporal Allocation Factors
HOUR1-HOUR288	8	Hourly Temporal Allocation Factors

TABLE B-3. SPATIAL ALLOCATION FACTOR SURROGATES FOR 1985 NAPAP CANADIAN AREA SOURCE EMISSIONS CATEGORIES

Category ID	Surrogate ID	Surrogate Indicator	Emissions Category Description
11000	4	Housing	Stationary Fuel Combustion - Residential Natural Gas
11200	4	Housing	Stationary Fuel Combustion - Residential Natural Gas Liquids
11300	4	Housing	Stationary Fuel Combustion - Residential Kerosene and Stove Oils
11400	4	Housing	Stationary Fuel Combustion - Residential Coal
11510	4	Housing	Stationary Fuel Combustion - Residential Distillate Oil
11520	4	Housing	Stationary Fuel Combustion - Residential Residual Oil
11610	4	Housing	Stationary Fuel Combustion - Residential Conventional Wood Stove
11620	4	Housing	Stationary Fuel Combustion - Residential Slow Combustion Stove
11630	4	Housing	Stationary Fuel Combustion - Residential Fireplace
11640	4	Housing	Stationary Fuel Combustion - Residential Wood Furnace
12100	6	Commercial Labor Force	Stationary Fuel Combustion - Commercial/Inst Natural Gas
12200	6	Commercial Labor Force	Stationary Fuel Combustion - Commercial/Inst Liquid Petroleum Gas
12300	6	Commercial Labor Force	Stationary Fuel Combustion - Commercial/Inst Kerosene Stove Oil
12400	6	Commercial Labor Force	Stationary Fuel Combustion - Commercial/Inst Coal
12510	6	Commercial Labor Force	Stationary Fuel Combustion - Commercial/Inst Distillate Oil
12520	6	Commercial Labor Force	Stationary Fuel Combustion - Commercial/Inst Residual Oil
13100	5	Industrial Labor Force	Stationary Fuel Combustion - Industrial Natural Gas
13200	5	Industrial Labor Force	Stationary Fuel Combustion - Industrial Natural Gas Liquids
13300	5	Industrial Labor Force	Stationary Fuel Combustion - Industrial Kerosene and Stove Oils
13400	5	Industrial Labor Force	Stationary Fuel Combustion - Industrial Coal
13510	5	Industrial Labor Force	Stationary Fuel Combustion - Industrial Distillate Oil
13520	5	Industrial Labor Force	Stationary Fuel Combustion - Industrial Residual Oil
14100	1	Population	Misc Power Generation - Natural Gas
14200	1	Population	Misc Power Generation - Heavy Fuel Oil
14300	1	Population	Misc Power Generation - Light Fuel Oil
14400	1	Population	Misc Power Generation - Misc Diesel Generator
21000	1	Population	Gasoline Vehicles - Automobiles
21100	1	Population	Gasoline Vehicles - Light Duty Trucks
21200	1	Population	Gasoline Vehicles - Heavy Duty Trucks
21300	1	Population	Diesel Vehicles - Light Duty Vehicles
21400	1	Population	Diesel Vehicles - Heavy Duty Vehicles
22100	1	Population	Off-Road Gasoline Vehicles - General
22140	1	Population	Off-Road Gasoline Vehicles - Snowmobiles
22210	1	Population	Off-Road Diesel Vehicles - Agricultural
22220	1	Population	Off-Road Diesel Vehicles - Construction
22230	1	Population	Off-Road Diesel Vehicles - Mining
22240	1	Population	Off-Road Diesel Vehicles - Manufacturing
22250	1	Population	Off-Road Diesel Vehicles - Forestry
22260	1	Population	Off-Road Diesel Vehicles - Public Administration
22270	1	Population	Off-Road Diesel Vehicles - Pipeline
23110	1	Population	Off-Highway Mobile Sources - Jet Aircraft
23120	1	Population	Off-Highway Mobile Sources - Turboprop Aircraft
23130	1	Population	Off-Highway Mobile Sources - Piston Engine Aircraft
23140	1	Population	Off-Highway Mobile Sources - Helicopter
23150	1	Population	Off-Highway Mobile Sources - Small Piston Aircraft
24100	1	Population	Off-Highway Mobile Sources - Railroad Diesel Oil

(continued)

TABLE B-3. (Continued)

Category ID	Surrogate ID	Surrogate Indicator	Emissions Category Description
25110	1	Population	Off-Highway Mobile Sources - Motorships Dockside
25120	1	Population	Off-Highway Mobile Sources - Steamships Dockside
25210	1	Population	Off-Highway Mobile Sources - Motorships Underwat
25220	1	Population	Off-Highway Mobile Sources - Steamships Underway
25310	1	Population	Off-Highway Mobile Sources - Gasoline Outboards
27110	1	Population	Gasoline & Diesel Mkting - Refining Storage Transfer
27111	1	Population	Gasoline & Diesel Mkting - Filling Vehicle Tanks
27120	1	Population	Gasoline & Diesel Mkting - Diesel Evaporation
27130	1	Population	Gasoline & Diesel Mkting - Station Storage Transfer
27140	1	Population	Gasoline & Diesel Mkting - Vapor Loss at Station (Tank)
27150	1	Population	Gasoline & Diesel Mkting - Transfer to Cars
27160	1	Population	Gasoline & Diesel Mkting - Spillage at Station
31300	1	Population	Solid Waste Incineration - Multiple Chamber
31500	1	Population	Solid Waste Incineration - Controlled Air
32100	8	Mining Labor Force	Solid Waste Incineration - Wood Waste Disposal
33100	7	Agricultural Labor Force	Slash Burning
47100	8	Mining Labor Force	Forest Fires
47200	4	Housing	Structural Fires
51000	6	Commercial Labor Force	Bakeries
52110	8	Mining Labor Force	Crude Oil Production - Evaporation of Hydrocarbons
53110	5	Industrial Labor Force	Clay Products Manufacturing - Dryer/Grinder
53120	5	Industrial Labor Force	Clay Products Manufacturing - Storage
53200	8	Mining Labor Force	Coal Industry - Coal Mining
53210	8	Mining Labor Force	Coal Industry - Coal Handling
53220	8	Mining Labor Force	Coal Industry - Overburden Removal (Fugitive)
53300	8	Mining Labor Force	Coal Industry - Transportation
53400	8	Mining Labor Force	Mining & Rock Quarrying
53410	8	Mining Labor Force	Mining & Rock Quarrying - Open Pit Mining
53420	8	Mining Labor Force	Mining & Rock Quarrying - Overburden Removal
53430	8	Mining Labor Force	Mining & Rock Quarrying - Underground Mining
53440	8	Mining Labor Force	Mining & Rock Quarrying - Concentrate Dryers
53450	8	Mining Labor Force	Mining & Rock Quarrying - Concentrate Transport
53500	5	Industrial Labor Force	Sand & Gravel Processing - General
53611	5	Industrial Labor Force	Stone Processing - Crushed Stone - Primary Crushing
53612	5	Industrial Labor Force	Stone Processing - Crushed Stone - Secondary Crushing
53613	5	Industrial Labor Force	Stone Processing - Crushed Stone - Conveying and Handling
53614	5	Industrial Labor Force	Stone Processing - Crushed Stone - Screening
53615	5	Industrial Labor Force	Stone Processing - Crushed Stone - Secondary Crushing (Fugitive)
53621	5	Industrial Labor Force	Stone Processing - Pulverized Stone - Primary Crushing
53622	5	Industrial Labor Force	Stone Processing - Pulverized Stone - Secondary Crushing
53624	5	Industrial Labor Force	Stone Processing - Pulverized Stone - Screening
53625	5	Industrial Labor Force	Stone Processing - Pulverized Stone - Fines Mill
53626	5	Industrial Labor Force	Stone Processing - Pulverized Stone - Storage Pile Losses
53627	5	Industrial Labor Force	Stone Processing - Pulverized Stone - Secondary Crushing (Fugitive)
53628	5	Industrial Labor Force	Stone Processing - Pulverized Stone - Recrushing
53631	5	Industrial Labor Force	Stone Processing - Building Stone - Cutting

(continued)

TABLE B-3. (Continued)

Category ID	Surrogate ID	Surrogate Indicator	Emissions Category Description
54100	1	Population	Asphalt Production - Drying
54200	1	Population	Asphalt Production - Fugitive
55100	1	Population	Concrete Batching
55200	1	Population	Concrete Batching - Fugitive Material Handling
56000	5	Industrial Labor Force	Plastic Fabrication
57100	8	Mining Labor Force	Wood Industry - Sawmill Production
57200	8	Mining Labor Force	Wood Industry - Plywood and Veneer Production
57300	8	Mining Labor Force	Wood Industry - Pulpboard Production
57400	8	Mining Labor Force	Wood Industry - Hardwood Production
61110	7	Agricultural Labor Force	Grain Milling/Handling - Terminal Elev - Shipping & Receiving
61120	7	Agricultural Labor Force	Grain Milling/Handling - Terminal Elev - Transfer & Conveying
61130	7	Agricultural Labor Force	Grain Milling/Handling - Terminal Elev - Cleaning
61140	7	Agricultural Labor Force	Grain Milling/Handling - Terminal Elev - Drying
61150	7	Agricultural Labor Force	Grain Milling/Handling - Terminal Elev - Headhouse
61160	7	Agricultural Labor Force	Grain Milling/Handling - Terminal Elev - Tripper (Gallery Belt)
61210	7	Agricultural Labor Force	Grain Milling/Handling - Terminal Elev - Shipping & Receiving
61220	7	Agricultural Labor Force	Grain Milling/Handling - Terminal Elev - Transfer & Conveying
61230	7	Agricultural Labor Force	Grain Milling/Handling - Terminal Elev - Headhouse
61240	7	Agricultural Labor Force	Grain Milling/Handling - Terminal Elev - Tripper (Gallery Belt)
61310	7	Agricultural Labor Force	Grain Milling/Handling - Process Elev - Receiving
61320	7	Agricultural Labor Force	Grain Milling/Handling - Process Elev - Precleaning & Handling
61330	7	Agricultural Labor Force	Grain Milling/Handling - Process Elev - Cleaning House
61340	7	Agricultural Labor Force	Grain Milling/Handling - Process Elev - Millhouse
61410	7	Agricultural Labor Force	Grain Milling/Handling - Priminal Elev - Shipping & Receiving
61420	7	Agricultural Labor Force	Grain Milling/Handling - Priminal Elev - Transfer & Conveying
61430	7	Agricultural Labor Force	Grain Milling/Handling - Priminal Elev - Headhouse
64000	7	Agricultural Labor Force	Fertilizer Application
64100	7	Agricultural Labor Force	Fertilizer Application - Ammonia Distributors
66100	7	Agricultural Labor Force	Animal Waste - Cattle Dung
66200	7	Agricultural Labor Force	Animal Waste - Pig Excrement
66300	7	Agricultural Labor Force	Animal Waste - Sheep Manure
70000	1	Population	General Solvent Use
71000	1	Population	Dry Cleaning
77000	1	Population	Application of Surface Coating - Trade/Sales Use
78200	5	Industrial Labor Force	Application of Surface Coating - Industrial Use
85100	5	Industrial Labor Force	Ferrous Foundries - Induction Furnace (Hot Melt)
85200	5	Industrial Labor Force	Ferrous Foundries - Cupola Furnace (Hot Melt)
85300	5	Industrial Labor Force	Ferrous Foundries - Electric Arc Furnace (Hot Melt)

NOTE: The surrogates corresponding to Oil Homes and Gas Homes were not used.

TABLE B-4. FILE FORMAT FOR THE EBCDIC 1985 CANADIAN SPATIAL ALLOCATION FILE

Record position		Column width	Format	Variable name	Description
First	Last				
1	2	2	I	STATE	AEROS State (Province) Code
3	6	4	-	-	Not used
7	11	5	I	SCC	Area Source Category Code
12	14	3	I	NGRID	Number of Grids in Province
15	18	4	I	NROW	Row of Grid Cell
19	22	4	I	NCOL	Column of Grid Cell
23	27	5	F5.4	NSAF[a]	Spatial Allocation Factor for Grid Cell[b]

[a]Implied decimal, with four digits to the right of the decimal place and one to the left.

[b]Spatial allocation factors are dimensionless fractions representing the portion of a province's land use for a specific spatial category in a grid cell.

Note: Columns 15 to 27 are repeated up to NGRID (900) times.

the process descriptions were not easily matched to specific profiles. In these cases, EPA assigned industry average default profiles or the overall average default profile. A list of the additional Canadian SCCs and the profile assignments applied to those SCCs is presented in Table B-5. Similarly, profiles were matched to all Canadian area source categories in order to facilitate speciation in FREDS. These profile assignments are shown in Table B-6.

Source category-profile matches for hydrocarbons were input to PSPLIT to create speciation factors suitable for the use with FREDS. Programs developed to manipulate U.S. particulate data were modified to accommodate Canadian profile assignments and used to create the particulate speciation factor files.

Unlike the U.S., the Canadian area source annual files contained emission estimates for four alkaline species (Na, K, Mg, Ca) in addition to TSP. Environment Canada requested that these annual particulate species be resolved by size fraction, rather than derive all PM species size combinations from TSP. Alliance subsequently modified its speciation programs to account for this methodology difference. Since some of the new Canadian area source speciation factors can equal unity, the SFF input format for speciation factors was charged from 'F8V8' to 'F8V7' to account for the possibility of a nonzero digit to the left of the decimal. All other PSPLIT and SFF formats remained the same as for the U.S.

Canadian annual area source hydrocarbon values were reported as THC rather than VOC. As a result, the Hydrocarbon Preprocessor was executed with all methane augmentation flags set to zero, allowing VOC to be calculated from input THC rather than vice versa.

REFERENCES

Shareef, G., W. Butler, L. Bravo, and M. Stockton. Air Emissions Species Manual Volume I - Volatile Organic Compound (VOC) Species Profiles. EPA-450/2-88-003a (NTIS PB88-225792), U.S. Environmental Protection Agency, Research Triangle Park, NC. April 1988.

Shareef, G., and L. Bravo. Air Emissions Species Manual Volume II - Particulate Matter (PM) Species Profiles. EPA-450/2-88-003b (NTIS PB88-225800). U.S. Environmental Protection Agency, Research Triangle Park, NC. April 1988.

TABLE B-5. ASSIGNMENT OF HYDROCARBON AND PARTICULATE SPECIATION PROFILES FOR EXTRA CANADIAN POINT SOURCE SCCS

Canadian SCC	THC profile	PM profile
10100104	1178	11201
10200692	3	26101
1020069	3	26101
10201499	0	13501
10299999	0	0
20100291	1001	34001
20100292	1001	34001
20200292	1001	34001
30102299	0	90002
30102702	0	90002
30102703	0	90002
30102799	0	0
30103005	0	90002
30300099	0	0
30300191	0	29101
30300192	0	29101
30300799	0	28401
30300905	16	90004
30501991	0	90013
30600195	9012	26101
30600299	9012	26202
30610099	9012	90014
30700194	9001	90015
30700196	9001	90015
30700201	9001	0
30700208	9001	0
30700290	9001	0
30700210	9001	0
30700399	0	0
30900360	0	90016
31000306	0	0
31000999	0	0
35001001	0	0
40300000	0	0
40301999	9024	0
50100103	122	17106
50100504	122	90001
50300199	9022	90001

TABLE B-6. ASSIGNMENT OF HYDROCARBON AND PARTICULATE SPECIATION PROFILES FOR CANADIAN AREA SOURCE CATEGORIES

SCC	Profile Assignment THC	TSP
11100	0195	26101
11200	0195	26101
11300	0002	13501
11400	1185	43201
11510	0002	13501
11520	0001	13501
11610	1084	42330
11620	1084	42330
11630	1084	42330
11640	1084	42330
12100	0003	26101
12200	0004	26101
12300	0002	13501
12400	1185	11201
12510	0002	13501
12520	0001	13501
13100	0003	26101
13200	0003	26101
13300	0002	13501
13400	1185	11201
13510	0002	13501
13520	0001	13501
14100	0003	26101
14200	0001	11501
14300	0002	11501
14400	0008	32202
21000	1101	31230
21100	1101	31230
21150	1101	31230
21200	1186	31102
21300	1201	32101
21400	1201	32202
22100	1101	31230
22140	1101	31230
22210	1201	32202
22220	1201	32202
22230	1201	32202
22240	1201	32202
22250	1201	32202
22260	1201	32202
22270	1201	32202
23110	1098	34001
23120	1099	34001
23130	1099	34001
23140	1099	34001
23150	1099	34001
23210	1098	34001
23230	1099	34001
23240	1099	34001
23250	1099	34001
23260	1099	34001
24100	1201	32202
25110	1201	32202
25120	1201	32202
25210	1201	32202
25220	1201	32202
25310	1186	31102
26100	0000	34002
26200	0000	34002
27110	1190	00000
27111	1190	00000
27120	1190	00000
27130	1190	00000
27140	1190	00000
27150	1100	00000
27160	1100	00000
31300	0122	17106
31500	0122	17106
32100	0122	17106
33100	0121	42301
41110	0000	41130
41120	0000	41130
42110	0000	41220
42120	0000	41220
42210	0000	41220
42220	0000	41220
42310	0000	41220
42320	0000	41220
43100	0000	41350
43200	0000	41350
44000	0202	90001
45100	0000	41350
45200	0000	41350
45300	0000	41350
45400	0000	41350
45500	0000	41350
46100	0000	41350
47100	0307	42320
47200	0000	42320
51000	9004	90002
52110	9012	33020
52120	9024	90014
53110	0000	90012
53120	0000	90012
53200	9011	21204
53210	9011	21204
53220	9011	21204
53300	9011	21204
53410	9011	90006
53430	9011	90006
53440	9011	90006
53450	9011	90006
53500	9011	90007
53611	9011	90007
53612	9011	90007
53613	9011	90007
53614	9011	90007
53615	9011	90007
53621	9011	90007
53622	9011	90008
53623	9011	90008
53624	9011	90008
53625	9011	90008
53626	9011	90008
53627	9011	90008
53628	9011	90008
53631	9011	90008
54100	9004	00000
54200	9004	00000
55100	0000	00000
55200	0000	00000
56000	9005	00000
57100	9013	22201
57200	1189	22301
57300	9013	22101
57400	9013	22201
61110	1201	21401
61120	9008	21401
61130	9008	21401
61140	9008	21401
61150	9008	21401
61160	9008	21401
61210	1201	21401
61220	9008	21401
61230	9008	21401
61240	9008	21401
61310	1201	21401
61320	9008	21401
61330	9008	21401
61340	9008	21401
61410	1201	21401
61420	9008	21401
61430	9008	21401
64000	0203	90003
64100	0203	25404
65000	0076	00000
66100	0203	90003
66200	0203	90003
66300	0203	90003
70000	0197	00000
71000	1196	00000
77000	1016	00000
78200	1016	00000
81000	0000	00000
85100	9009	28201
85200	9009	28202
85300	9009	28304

APPENDIX C

DEVELOPMENT OF ALLOCATION FACTORS FOR NATURAL SOURCES

APPENDIX C

DEVELOPMENT OF ALLOCATION FACTORS FOR NATURAL SOURCES

INTRODUCTION

A significant amount of research on natural source emissions in the United States has been conducted by the National Oceanic and Atmospheric Administration (NOAA) for NAPAP's Task Group on Atmospheric Chemistry (Task Group II) and EPA's Atmospheric Research and Exposure Assessment Laboratory (AREAL). For the 1985 NAPAP Version 2 Emissions Inventory, emissions of alkaline particulate matter were available in a format readily adaptable to the NAPAP inventory.

Emissions inventories for alkaline particulate matter from natural sources were developed for three categories: unpaved roads, wind erosion and dust devils. Particulate matter from paved roads are not included in the 1985 NAPAP inventory. Data were provided by Task Group II for total particulate mass and the mass of total calcium (Ca), magnesium (Mg), sodium (Na) and potassium (K). Data sources for calculation of annual and resolved natural particulate emissions include field measurements, AP-42 (EPA, 1985), and particulate matter species profiles (Shareef and Bravo, 1988). Unpaved road emissions were calculated at the county level by Barnard et al (1986a, 1986b, 1986c, 1987). Wind erosion and dust devil emissions estimates were provided by Task Group II for major land resource areas (MLRAs). These emissions estimates were resolved to the county level by EPA. Temporal, spatial and species resolution of the natural particulate emissions were derived from information provided by Task Group II and EPA.

Environment Canada also supplied natural source particulate emissions estimates from unpaved roads and wind erosion at the Provincial level. In addition, Environment Canada developed emissions estimates for total and alkaline particulate matter from paved roads. Temporal, spatial and species resolution were supplied by Environment Canada. A summary of U.S. and Canadian natural particulate categories included in the 1985 Version 2 inventory is provided in Table C-1.

TEMPORAL ALLOCATION FACTORS

Temporal allocation factors were developed individually for each of the natural source categories in the United States and Canada. Temporal factors derived for each source category at varying levels of specificity were

TABLE C-1. NATURAL ALKALINE PARTICULATE CATEGORIES INCLUDED IN THE 1985 NAPAP EMISSIONS INVENTORY (VERSION 2.0)

	SCC	Category description
U.S.		
	901	Unpaved Road Travel
	902	Wind Erosion, Natural and Agricultural Lands
	903	Dust Devils
Canadian		
	41110	Dust - Paved Roads - Vehicles
	41120	Dust - Paved Roads - Trucks
	42110	Dust Unpaved Roads - Vehicles - Treated Gravel
	42120	Dust Unpaved Roads - Trucks - Treated Gravel
	42210	Dust Unpaved Roads - Vehicles - Untreated Gravel
	42220	Dust Unpaved Roads - Trucks - Untreated Gravel
	42310	Dust Unpaved Roads - Vehicles - Earth Roads
	42320	Dust Unpaved Roads - Trucks - Earth Roads
	43200	Agricultural - Erosion from Crops

concatenated to form a natural source Temporal Allocation Factor File (TAFF) for U.S. natural source particulates. Canadian natural source temporal profiles were supplied by Environment Canada and are included in the Canadian area source Temporal Allocation Factor File. The appropriate linker variable was created in the Canadian annual natural source file for correspondence between the emissions file and the TAFF.

Unpaved road temporal profiles available in the U.S. area source TAFF were used to temporally allocate U.S. unpaved road emissions. These factors are SCC-specific and are based on U.S. Department of Transportation data for light duty vehicles on rural roads.

County-specific temporal profiles for wind erosion emissions in the United States are based on temporal information supplied by Task Group II. Seasonal fractions were calculated for each of the alkaline species and total particulates for each county by summing the monthly emissions for a season and dividing the seasonal total by the annual emissions. The seasonal values for total particulates and the alkaline components were combined to calculate average seasonal values for all (U.S.) particulate emissions from wind erosion. The diurnal profile for wind erosion, as recommended by Task Group II, was derived from a figure by Wigner and Peterson (1987) showing the occurrence of blowing dust by time of day. Daily factors were assumed to be uniform.

Quality control checks were performed on the wind erosion county specific seasonal profiles to assure the quality and compatibility of the factors. County codes were matched to those in the U.S. annual natural source emissions file. Any nonmatches were adjusted to assure complete temporal allocation. In addition, all seasonal and diurnal fractions were checked to ensure that they summed to unity.

Category-specific seasonal factors for U.S. dust devil emissions were based on data recommended by Task Group II and from unpublished data from a National Park Service Study (Contract No. USDICX-0001-3-0056, W. Malm, NPS Project Manager). The seasonal distribution of dust devils peaks between June 1 and September 1, decreases linearly from September 1 to October 15, falls to zero between October 15 and April 15, and finally begins a linear rise from April 15 to June 1. The diurnal profile recommended by Task Group II from Snow and McClelland (1988) shows maximum activity from 11 a.m. to 3 p.m., a linear decrease from 3 p.m. to 4 p.m., zero activity from 4 p.m. to 10 a.m., and a linear increase from 10 a.m. to 11 a.m.

The temporal profiles for each category for each scenario were concatenated to form the natural source TAFF. As a final check on the temporal data, seasonal and hourly fractions were totaled to verify that they summed to unity.

SPATIAL ALLOCATION FACTORS

The land area surrogate available in the U.S. spatial fraction file was used for spatial allocation of U.S. natural source emissions. The gridded spatial fractions were matched to the natural source Surrogate Selection File to generate a natural source Spatial Allocation Factor File (SAFF).

Spatial allocation factors for Canadian natural particulates were provided by Environment Canada. Paved road particulate emissions were allocated using population as a surrogate and the unpaved road and wind erosion categories were allocated using the agricultural labor force surrogate.

SPECIATION FACTORS

The NAPAP Task Group II research results related to natural alkaline particulate included estimates of total mass and the total mass of the alkaline species for limited size ranges. These estimates were divided into the appropriate size and reactivity fractions to provide estimates that were consistent with the anthropogenic particulate data. The measured data for unpaved road dust indicated that 24 percent of the total mass was included in the 10 micron and smaller size fraction. The total TSP mass was estimated by multiplying the less than 10 micron size fraction by 4.17, the inverse of the 24 percent fraction.

Data that were available in AP-42 suggest that the less than 10 micron size fraction is 36 percent. Estimates of size fractions for unpaved road dust in size ranges of less than 2.5 micron; less than 5.0 micron; less than 10 micron; less than 15 micron and less than 30 micron are also included in AP-42. These data were plotted and a linear regression was applied to determine the fraction of particulate in the less than 6.0 micron size range.

Reactivity fractions were obtained from the *Air Emissions Species Manual Volume II* (Shareef and Bravo, 1988). The AP-42 size fractions were scaled by the ratio of 0.24/0.36 to develop estimates of the size fraction required for the NAPAP inventory. The same size fractions were applied to both TSP and the individual alkaline components. These size fractions were used in the speciation of all three natural source categories. The speciation factors applied to the NAPAP natural source particulate data are listed in Table C-2.

Size fractions for Canadian natural particulates were available in the Canadian area source Speciation Factor File (SFF) and the alkaline fractions were obtained from profiles for the natural source categories that were included in the *Air Emissions Species Manual.*

TABLE C-2. SPECIATION FACTORS FOR U.S. NATURAL ALKALINE PARTICULATES

Species	Reactive fraction	0-2.5 um fraction	2.5-6.0 um fraction	6.0-10.0 um fraction	2.5-10.0 um fraction
TSP	NA	0.0207	0.090	0.129	NA
Sodium (Na)	0.0	0.0207	NA	NA	0.2194
Potassium (K)	0.0	0.0207	NA	NA	0.2194
Calcium (Ca)	0.5	0.0207	NA	NA	0.2194
Magnesium (Mg)	0.5	0.0207	NA	NA	0.2194

REFERENCES

U.S. Environmental Protection Agency. Compilation of Air Pollutant Emission Factors, Fourth Edition, AP-42 Volume 1, (GPO No. 055-000-00251-7), Research Triangle Park, NC. 1985.

Shareef, G. and L. Bravo. Air Emissions Species Manual Volume II - Particulate Matter (PM) Species Profiles. EPA-450/2-88-003b (NTIS PB88-225800). U.S. Environmental Protection Agency, Research Triangle Park, NC. April 1988.

Barnard, W.R., G.J. Stensland, and D.F. Gatz, 1986a. Alkaline Materials Flux From Unpaved Roads: Source Strength, Chemistry and Potential for Acid Rain Neutralization, Water Air and Soil Pollution, 30, p. 285-293.

Barnard, W.R., G.J. Stensland, and D.F. Gatz, 1986b. Development of Alkaline Emission Flux Estimates From Unpaved Roads: Problems and Data Needs for Modeling Potential Acid Rain Neutralization, Paper 86-30.4, Proceedings 79th Annual Meeting of the Air Pollution Control Association, Minneapolis, MN.

Barnard, W.R., D.F. Gatz, and G.J. Stensland, 1986c. Elemental Chemistry of Unpaved Surface Materials, Paper 86-21.2, Proceedings of the 79th Annual Meeting of the Air Pollution Control Association, Minneapolis, MN.

Barnard, W.R., D.F Gatz, and G.J. Stensland, 1987. Evaluation of Potential Improvements in the Estimation of Unpaved Road Fugitive Emission Inventories, Paper 87-58.1, Proceedings of the 80th Annual Meeting of the Air Pollution Control Association, New York, NY.

Wigner, K. and R. Peterson. Synoptic Climatology of Blowing Dust on the Texas South Plains, 1947-84. Journal of Arid Environments, 13, 199-209. 1987.

Snow, J. T. and T. McClelland. Dust Devils at White Sands Missile Range, New Mexico, USA. J. Meteoro, 13, 156-164. 1988.

APPENDIX D
DESCRIPTION OF SEASONAL ELECTRIC UTILITY FACTORS

E. H. PECHAN & ASSOCIATES, INC.
5537 Hempstead Way
Springfield, VA 22151
(703) 642-1120

December 6, 1988

Mr. Mark Saeger
Alliance Technologies, Inc.
500 Eastowne Drive
Chapel Hill, NC 27514

Dear Mr. Saeger:

This letter transmits a description of the seasonal electric utility factors which we have recently developed.

The file itself is in SAS format on the EPA IBM 3090 mainframe. It has the name EXPNAPA.NAPAP.UTILITY.SEASONAL.SASDATA. The SAS data set name to use in this file is UTILSEAS. The specific contents are documented in Exhibit 2 to the enclosure.

Feel free to contact me if you have any questions on this information or how it was developed.

Sincerely,

Edward H. Pechan

Enclosure

cc: David Fratt, Alliance
Rob Lagemann
David Mobley

Calculating Season Activity Levels for Electric Utilities

Seasonal activity factors for inclusion in the NAPAP inventory were estimated for electric utilities for the year 1985. The activity factors were based primarily on data collected by the Department of Energy.

The major source of data contributing to the seasonal estimates was Energy Information Administration Form 759. This form collects monthly fuel use data by plant and fuel type (and prime mover). These monthly data were aggregated to season by plant and four fuel types (coal, residual oil, distillate oil, and natural gas). The following seasonal definitions were used:

Winter	December, January, February
Spring	March, April, May
Summer	June, July, August
Fall	September, October, November

For each plant, a surrogate measure for "other" fuel was defined based on the sum of the four fuels indicated above. The "other" category represents minor fuels used at a few plants such as petroleum coke and process gas. These minor fuels, included in NAPAP but not reported in Form 759, were assigned seasonal allocations averaged from the usage of the four main fuel types.

NAPAP Source Classification Codes (SCC) were used to determine applicable fuel types based on the first six digits. The allocation was as follows:

101001-101003	Coal
101004	Residual Oil
101005	Distillate Oil
101006	Natural Gas
101007	Other

The list of applicable NAPAP plants was selected based on the first three digits of the SCC being 101 (electric utility boiler). These plants were then matched to the data derived from the Form 759 data. Matching was performed using a hierarchical approach as listed below.

Plant-fuel

State-fuel

State-all fuels

In the case of Texas, no plant-level data were available in the NAPAP inventory. As a result, all of the SCCs were matched at the state-fuel level. Some plants could not be matched on a state level because, although they reported coal as a fuel, for example, they reported no coal burned.

Table 1* reports the results of the matching of NAPAP plants to Form 759 fuel use. For coal, almost 90 percent of total fuel use from NAPAP was matched at the plant level. Of the remaining amount, the vast majority was accounted for by the Texas plants for which NAPAP did not provide plant-level information. For residual oil, the match ratio was over 98 percent. It was 62 percent for distillate oil and 45 percent for natural gas. State-level matches were required for less than 0.5 percent of fuel use for all fuels except distillate oil, which had a state-level match figure of 8.2 percent.

Most nonmatches occurred due to definitional differences between NAPAP and EIA 759 data. For EIA 759, electric utilities are defined as units which provide electricity to the common grids. The NAPAP definition of electric utilities (SCC 101) included a number of units which did not meet this criterion. Even when NAPAP SCC 101 units which did not have the electric utility Standard Industrial Code (4911) were deleted, some units remained in NAPAP which would clearly not be classed as utilities by DOE. The number of such units was small, however, as was their share of total fuel use.

Table 2 provides an alphabetical list of variables and attributes contained in the data set below:

EXPNAPA.NAPAP.UTILITY.SEASONAL.SASDATA

The data set name to use in this file is UTILSEAS.

(*) Table D-1.

TABLE D-1. METHODS USED TO ALLOCATE FUEL USE TO SEASONS

Table 1

Methods Used to Allocate Fuel Use to Seasons

	Number of Plants	Fuels Used	% of Fuels Used
Fuel-specific matches			
Coal (1000 tons)			
Plant-fuel			
Texas (see note)	552	617,442	89.3
State-fuel	74	72,639	10.5
Totals	10	1,584	0.2
	636	691,665	
Residual Oil (million gallons)			
Plant-fuel			
Texas (see note)	189	6,328	98.3
State-fuel	72	90	1.4
Totals	27	19	0.3
	288	6,437	
Distillate Oil (million gallons)			
Plant-fuel			
Texas (see note)	270	303	62.2
State-fuel	72	144	29.6
Totals	41	40	8.2
	383	487	
Natural Gas (billion cubic feet)			
Plant-fuel			
Texas (see note)	341	1,656	45.3
State-fuel	72	1,988	54.4
Totals	24	9	0.2
	437	3,653	
Other fuels			
Plant-fuel			
Texas (see note)	48		
State-fuel	0		
Totals	7		
	55		
Not fuel-specific matches			
Other fuels			
State total	2		

Note: No plant-level data were available from the NAPAP inventory for Texas